User Guide Version 6.1

Volume IV: Examples

"Resolution of partial differential equations is more about art than science".

Apocryphal quotation from Numerical Recipes in Fortran

"2 + 2 = 4 except for large values of 2"

Anonymous

"42"

Douglas Adams

Edited by: MICRESS group

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1 Introduction

The software MICRESS® (MICRostructure Evolution Simulation Software) is developed for time- and space-resolved numerical simulations of solidification, grain growth, recrystallisation or solid state transformations in metallic alloys. MICRESS® covers phase evolution, solutal and thermal diffusion and transformation strain in the solid state. It enables the calculation of microstructure formation in time and space by solving the free boundary problem of moving phase boundaries.

The microstructure evolution is governed essentially by thermodynamic equilibria, diffusion and curvature. In case of multicomponent alloys, the required thermodynamic data can either be provided to MICRESS® in the form of locally linearized phase diagrams, or by direct coupling to thermodynamic data sets via a special TQ interface, developed in collaboration with Thermo-Calc™ AB, Stockholm.

MICRESS® is based on the multi-phase-field method which defines a phase-field parameter for each phase involved. The phase-field parameter describes the fraction of each phase as a continuous function of space and time. Each single grain is mapped to a distinct phase-field parameter and is treated as an individual phase. A set of coupled partial differential equations is formed which describes the evolution of the phase-field parameter, together with concentration, temperature, stress and flow fields. The total set of equations is solved explicitly by the finite difference method on a cubic grid.

2D and 3D simulations are possible. The size of the simulation domain, the number of grains, phases and components is restricted mainly by the available memory size and the CPU speed.

Suggestions for improvements of the manual or comments on the manual are highly welcome to documentation@micress.de.

MICRESS® handles:

- 1-, 2- and 3-dimensional calculation domains
- arbitrary number of components, phases and grains

- solid-solid and solid-liquid interaction
- anisotropy of grain boundaries, mobility and energy

MICRESS® supports:

- coupling to thermodynamic database (via the TQ-interface of Thermo-Calc™)

In the present **MICRESS® User Guide Part IV: "MICRESS** Examples" you will find:

- an overview of available MICRESS® examples
- a short description of the different examples, their scope and the respective simulation conditions/parameters
- some visualized results for each example

Major scope of this manual is to provide a quick overview over the different examples and different MICRESS features used to run them without the need of visualizing the results with DP_MICRESS or stepping deeper into the respective driving files.

A description of the phase-field phenomenology and theoretical background can be found in *MICRESS Vol. 0*: **MICRESS Phenomenology**. *MICRESS Vol. I*: **Installing MICRESS** provides information about the installation of the software and explains how to verify successful installation with the help of simple examples. *MICRESS Vol. II*: **Running MICRESS** offers an overview of the input file structure, as well as theoretical and practical information on metallurgical processes, numerical modelling using the phase-field model and troubleshooting when starting a simulation. It provides useful hints on how to build the input file according to the process to be simulated. *MICRESS Vol. III*: **MICRESS Post-processing** explains the possibilities for analysing MICRESS output results.

2 What's new?

This section will be regularly up-dated with new examples for new features of MICRESS once they have become established examples.

A substantial revision of the present examples along with the description of further instructive examples is intended to be part of the next release.

3 Examples Overview

MICRESS® examples are located in the MICRESS® installation directory or can be downloaded from the web (www.micress.de). They do not cover the entire range of applications of the software, but treat some typical cases and can be used as starting points for other purposes. They also do not exploit the full complexity of the MICRESS software, which has already successfully been applied to technical alloy systems with more than 14 different thermodynamic phases, but rather demonstrate its basic features on the basis of simple examples.

The following tables give an overview of the features covered in the examples. They cover two examples categories. The first, table 1, comprises “solid state transformation” examples, where as the second, table 2, is dedicated to “solidification” examples.

Example		GammaAlpha_Pearlite_dri	GammaAlpha_PARATQ_dri	GammaAlpha_PARA_dri	GammaAlpha_NPLE_dri	GammaAlpha_dri	GammaAlpha_TQ_dri	GammaAlpha_Stress_dri	GammaAlpha_NPLE_dri	GammaAlphaCementite_TQ_dri	GammaAlphaCementite_LinTQ_dri	Grain_Growth_dri	Grain_Growth_Particle_Pinning_dri	Grain_Growth_Solute_Drag_dri	Grain_Growth_Solute_Drag_dG_dri	Grain_Growth_Profiles_dri	TQ_Ripening_dri	Stress_dri	ReX_1_dri	ReX_2_dri	ReX_3_dri	ReX_4_dri	ReX_5_dri	Antitroppoy	AlSi_antitrap_dri	Grain_Growth_triple_dri	
		01	02	03	04	05	06	07	08	09	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26
alloy						Fe-C-Mn	Fe-C-Mn	Fe-C-Mn	Fe-C-Mn	Fe-C-Mn	Fe-C-Mn						Al-Ag										
transformation						solid state transformation	solid state transformation	solid state transformation	solid state transformation	solid state transformation	solid state transformation	grain growth	grain growth	grain growth	grain growth	grain growth	ripening	(stress)	recrystallisation	recrystallisation	recrystallisation	recrystallisation	recrystallisation				
concentration coupling						X	X	X	X	X	X						X	X									
temperature coupling																											
only phase field												X	X	X	X	X			X	X	X	X	X				
stress field								X										X									
recrystallisation																				X	X		X				
dimension	1D																										
	2D					X	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X				
	3D							X																			

time step	automatic					X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X				
	manual																										
initial	directional																										
	equiaxed					X	X	X	X	X		X	X	X			X		X	X	X	X	X				
microstructure	deterministic					X	X		X	X	X							X	X	X		X					
	random							X								X	X				X		X				
	from file											X	X	X	X												
	voronoi					X	X	X	X	X	X					X	X	X	X	X	X	X	X				
	stochiometric phases							X		X	X																
nucleation model	types of seeds					X	X	X	X	X	X									X		X	X				
	seed density																										
	seed undercooling					X	X	X	X	X	X									X		X	X				
	restart option					X	X	X	X	X	X	X	X	X	X	X												
thermodynamic databases	thermodynamic coupling						X		X	X	X					X	X										
	& diffusion data									X	X																
anisotropy model	cubic															X	X		X	X	X	X	X				
	hexagona																										

	faceted																										
	antifaceted																										
	misorientation																			X	X	X	X				
far field approximation	1d far field																										
far field approximation	1d field for temperature coupling																										
	moving frame																										
	latent heat															X											
literface mobility models	solute drag													X													
literface mobility models	particle pinning												X														
read in data files	mobility													X	X	X											
read in data files	enthalpy																										
read in data files	heat capacity																										
read in data files	heat conductivity																										
read in data files	interfacial energy																										
read in data files	temperature trend															X											

Table 1 Overview of the "solid state transformation" features covered in the MICRESS examples

Example		Delta_Gamma_dri	AlCu_dri	AlCu_Equiaxed_dri	AlCu_Temp1d_dri	P_Peak_1D_dri	P_Peak_2D_dri	TQ_Eutectic_dri	Temperature_dri	AlCu_LinTQ_dri	AlSi_antitrap_dri	Antitroppoy_dri															
		01	02	03	04	05	06	07	08	09	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26
alloy		Fe-C-Mn	Al-Cu	Al-Cu	Al-Cu	Fe-C-Mn-P-Si	Fe-C-Mn- P-Si	Al-Ag																			
transformation		solidification	solidification	solidification	solidification	segregation	segregation	solidification	(temperature)																		
concentration coupling		X	X	X	X	X	X	X																			
temperature coupling									X																		
only phase field																											
stress field																											
recrystallisation																											
dimension	1D				X	X																					
	2D	X	X	X				X	X																		
	3D																										

time step	automatic	X	X	X	X	X	X	X	X																		
	manual							X	X																		
initial	directional	X	X		X	X																					
	equiaxed			X			X																				
microstructure	deterministic	X	X	X	X	X		X	X																		
	random						X		X																		
	from file																										
	voronoi						X																				
	stochiometric phases																										
nucleation model	types of seeds	X		X	X	X	X																				
	seed density			X																							
	seed undercooling	X			X	X	X																				
	restart option	X	X	X	X	X	X	X	X																		
thermodynamic databases	thermodynamic coupling	X	X	X	X	X	X	X	X																		
	& diffusion data				X	X		X	X																		
anisotropy model	cubic	X	X	X	X	X	X																				
	hexagona																										

	faceted																										
	antifaceted																										
	misorientation																										
far field approximation	1d far field	X	X																								
far field approximation	1d field for temperature coupling																										
far field approximation	moving frame	X	X																								
far field approximation	latent heat			X			X																				
literface mobility models	solute drag																										
literface mobility models	particle pinning																										
read in data files	mobility																										
read in data files	enthalpy																										
read in data files	heat capacity																										
read in data files	heat conductivity																										
read in data files	interfacial energy																										
read in data files	temperature trend																										

Table 2 Overview of the "solidification" features covered in the MICRESS examples

4 "Delta-Gamma"

4.1 Description

"Delta_Gamma_dri" is a 2D-simulation of the directional solidification of a ternary steel model alloy containing carbon and manganese. The simulation shows the solidification of a δ-phase dendrite and the subsequent peritectic reaction to the γ-phase. The simulation is performed as concentration-coupled and makes use of the 1d far field approximation and the moving frame option. It is coupled to Thermo-Calc™.

name dri file	Delta_Gamma.dri
alloy system	Fe-C-Mn (Steel.Ges5)
composition	98 at% Fe 1 at% C 1 at% Mn
transition	solidification, peritectic transformation

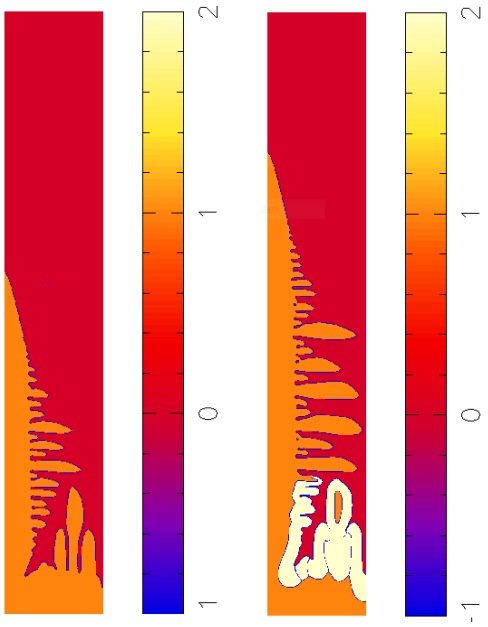


Figure 4.1. Example Delta_Gamma.phas: dendritic solidification at a time of 25 s (left) and peritectic reaction at a time of 32.5 s (right)

4.2 Simulation conditions

name dri file	Delta_Gamma.dri
dimension	2D
grid size	145x1500 cells
grid spacing	1µm
interface thickness	4 cells
boundary conditions	East: symmetric West: symmetric bottom: insulated top: fixed
solid phases:	Two solid phases: δ phase, γ phase
grain input	deterministic placement of 1 grain of δ-phase (round r = 0,0; position x = 0,5 , z = 0,5; stabilisation of the grain) further nucleation: γ-phase: seed position: interface; curvature undercooling; max. 5 seeds, ΔT = 1 K, rotation angle -5° to 5°; between 1765 K and 1700 K temperature conditions: T_0=1786 K; G = 250 K/cm; dT/dt = -1 K/s
output	files: restart, phases, average table fraction, interface, driving force, concentrations (C, Mn) times: -> fixed output at 0,01 s, 1,0 s and 2,5 s -> from 2,5 s to 35 s output every 2,5 s (linear step) -> from 35 s to 50 s output every 5,0s (linear step)
special features	-> concentration coupling -> 1d far field diffusion approximation (500 cells, distance from the front 200 µm) -> thermodynamic coupling (GES-file: Steel.GES5) -> moving frame (distance from the upper boundary 200 µm)

Table 3 Example Delta-Gamma: simulation conditions/parameters

4.3 Visualisation of the results

- Solidification sequence is presented by the .phas-output (-1: interface; 0: liquid; 1: δphase; 2: γphase)

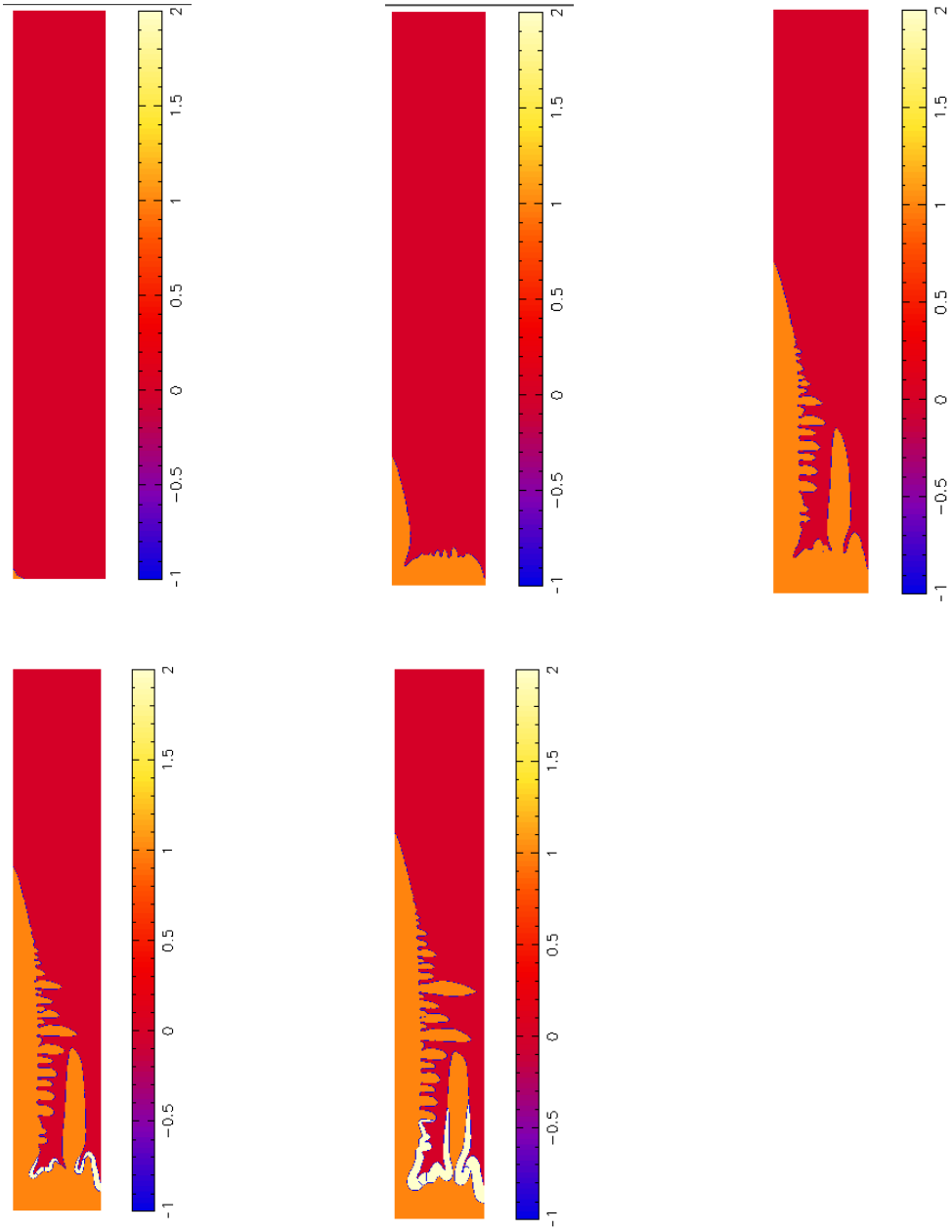


Figure 4.2. The Delta-Gamma solidification sequence at 1, 12.5, 25, 27.5 and 30 secs.

A preset δ-ferrite grain (lower left corner of upper left picture) grows dendritically in a temperature gradient (bottom cooling). A γ-austenite grain nucleates (lower left picture) and the peritectic reaction/transformation proceeds (lower row)

- Concentration of carbon (C) and Manganese (Mn)

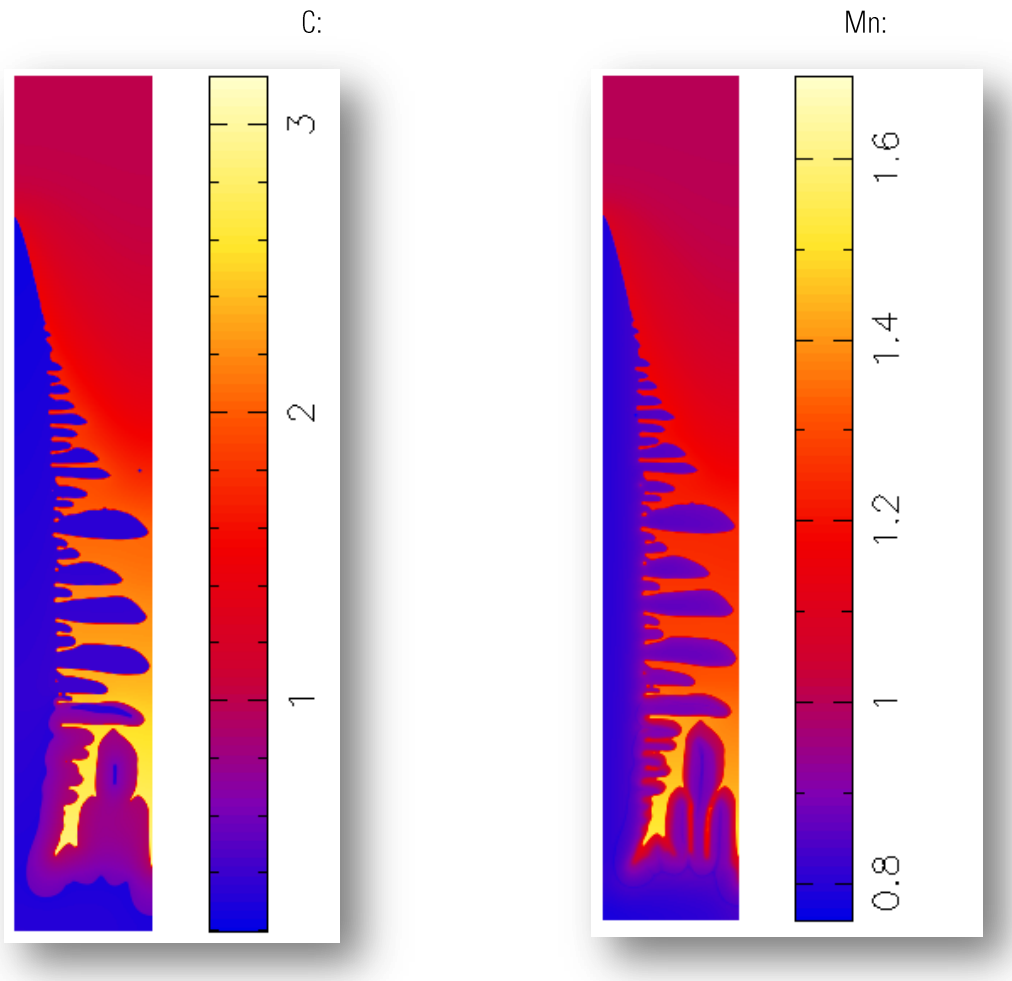


Figure 4.3 The concentrations fields for C (Delta_Gamma.conc1) and Mn(Delta_Gamma.conc2) for t=35s

5 "Aluminium-Copper"

5.1 Description

The three examples "Aluminium Copper" show the 2D solidification of a binary aluminium copper alloy. The "AlCu_dri" example corresponds to a directional solidification situation, whereas "AlCu_Equiaxed_dri" and "AlCu_Temp1d_dri"- describe equiaxed solidification.

All three examples are concentration-coupled with Thermo-Calc™ coupling. "AlCu_Equiaxed_dri" and "AlCu_Temp1d_dri" provide an example of the use of the "seed-density" nucleation model. Additionally "AlCu_Temp1d_dri" demonstrates the read-in of data files for temperature-dependent mobilities and latent heat as well as the use of the far field approximation for temperature coupling and release of latent heat. Another feature of this example is the use of categorized seeds.

name dri file	AlCu_dri.txt AlCu_Equiaxed_dri.txt AlCu_Temp1d_dri.txt
alloy system	Al-Cu (Al_Cu.Ges5)
composition	97 at% Al 3 at% Cu
transition	solidification

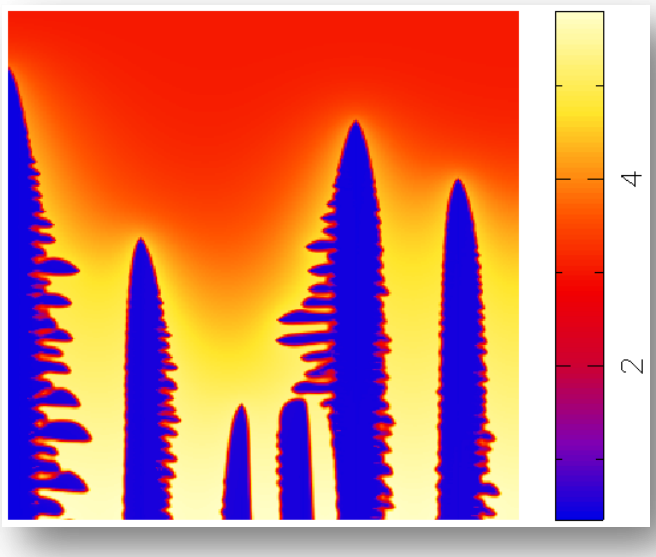


Table 4 Aluminium-Copper examples

5.2 Simulation conditions

name dri file	AlCu_dri.txt		AlCu_Equiaxed_dri.txt	AlCu_Temp1d_dri.txt
dimension	2D			
grid size	300x300 cells			200x200 cells
grid spacing	2µm			0.5µm
interface thickness	4 cells			3.5 cells
boundary conditions BCs				
phase field BCs	East:	symmetric	periodic	periodic
	West:	symmetric	periodic	periodic
	bottom:	symmetric	periodic	insulation
	top:	symmetric	periodic	insulation
concentration field BCs	East:	symmetric	periodic	periodic
	West:	symmetric	periodic	periodic
	bottom:	symmetric	periodic	insulation
	top:	fixed	periodic	insulation
solid phases:	1 solid phase: fcc_A1			2 solid phases: fcc_A1, AlCu_THETA
grain input	deterministic placement			
	1 grain of fcc_A1-phase (round r = 5; position: x = 0, z = 0; stabilisation of the grain)		0 grains at the beginning	
	further nucleation: NO		further nucleation: enabled	
	----------		seed position: bulk seed density nucleation model applied	
			integer for randomization: 13	integer for randomization: 111
			max. 1000 simultaneous nucleations	
	temperature conditions: T_0=912 K; G = 200 K/cm; dT/dt = -10 K/s		temperature conditions: T_0=915 K; G = 0 K/cm; Heat flow [J/s*cm^3]: -50.000	temperature conditions: T_0=950K Temp-field from file
	latent heat: NO		latent heat 3D enabled	
output	files: restart, grains, phases, fraction, average fraction table, interface, driving force, mobility, curvature, interface velocity, grain time, concentration, reference phase concentration, orientation, orientation time, linearization, monitoring outputs			
				relinearisation
	times: automatic output; from 0 s to 2 s output every 0.1 s (linear step)			times: fixed output at 0.03 s; from 0.03 s to 0.05 s output every 0.003 s (linear step) from 0.05 s to 0.4 s output every 0.01 s (linear step)
special features	concentration coupling			
	1d far field diffusion approximation (30 cells, distance from the front 60 µm)		NO 1d far field diffusion approximation	
	thermodynamic coupling (GES-file: Al_Cu.GES5)			
	moving frame (distance from the upper boundary 60 µm)		NO moving frame	

Table 5 Overview of Aluminum-Copper example simulation conditions

5.3 Visualisation of the results

5.3.1 Concentration

- AlCu_dri.txt

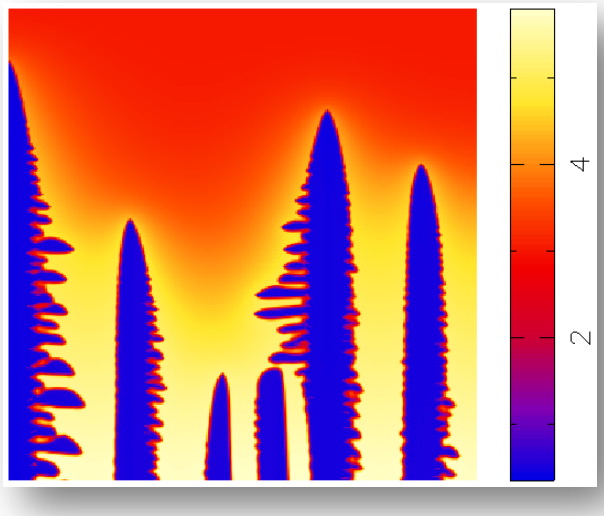


Figure 5.1. Concentration conc1 (Cu) at t=2s for driving file AlCu_dri.txt

- AlCu_Equiaxed_dri.txt

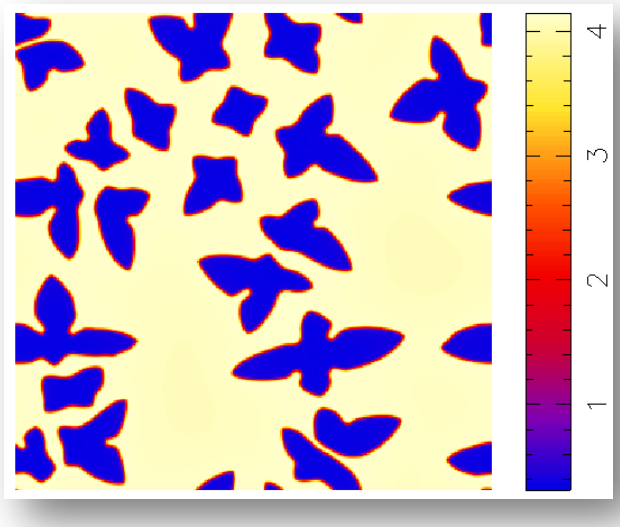
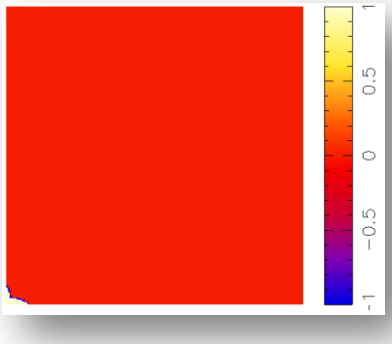


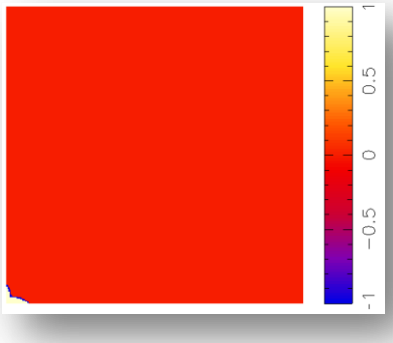
Figure 5.2. Concentration conc1 (Cu) at t=2s for driving file AlCu_Equiaxed_dri.txt

5.3.2 Solidification sequence presented by the .phas-output

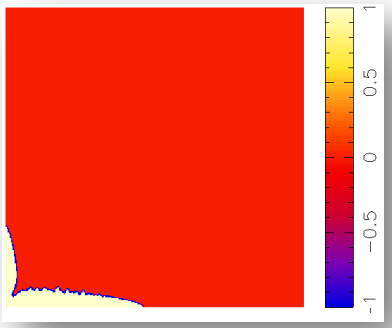
- AlCu_dri.txt (-1 → interface; 0 → liquid; 1 → fcc_A1 phase)



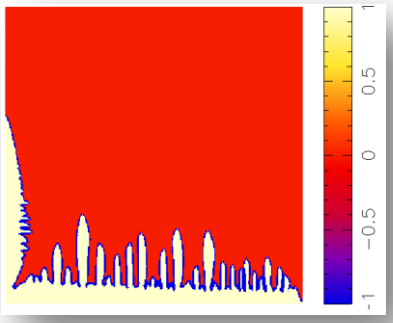
t=0s



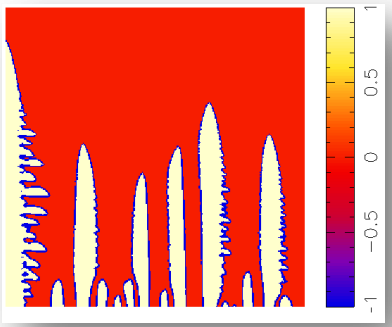
t=0.1s



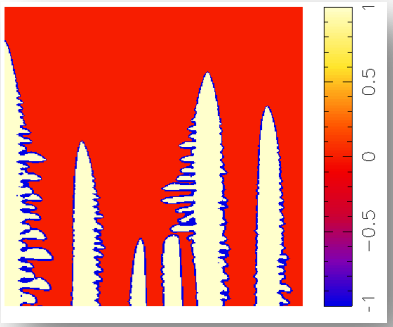
t=0.5s



t=1.0s



t=1.5s



t=2.0s

Figure 5.3. The solidification path: AlCu_dri.txt. Example: AlCu_phas

- AlCu_Equiaxed_dri.txt (-1 ⟶ interface; 0 ⟶ liquid; 1 ⟶ fcc_A1 phase)

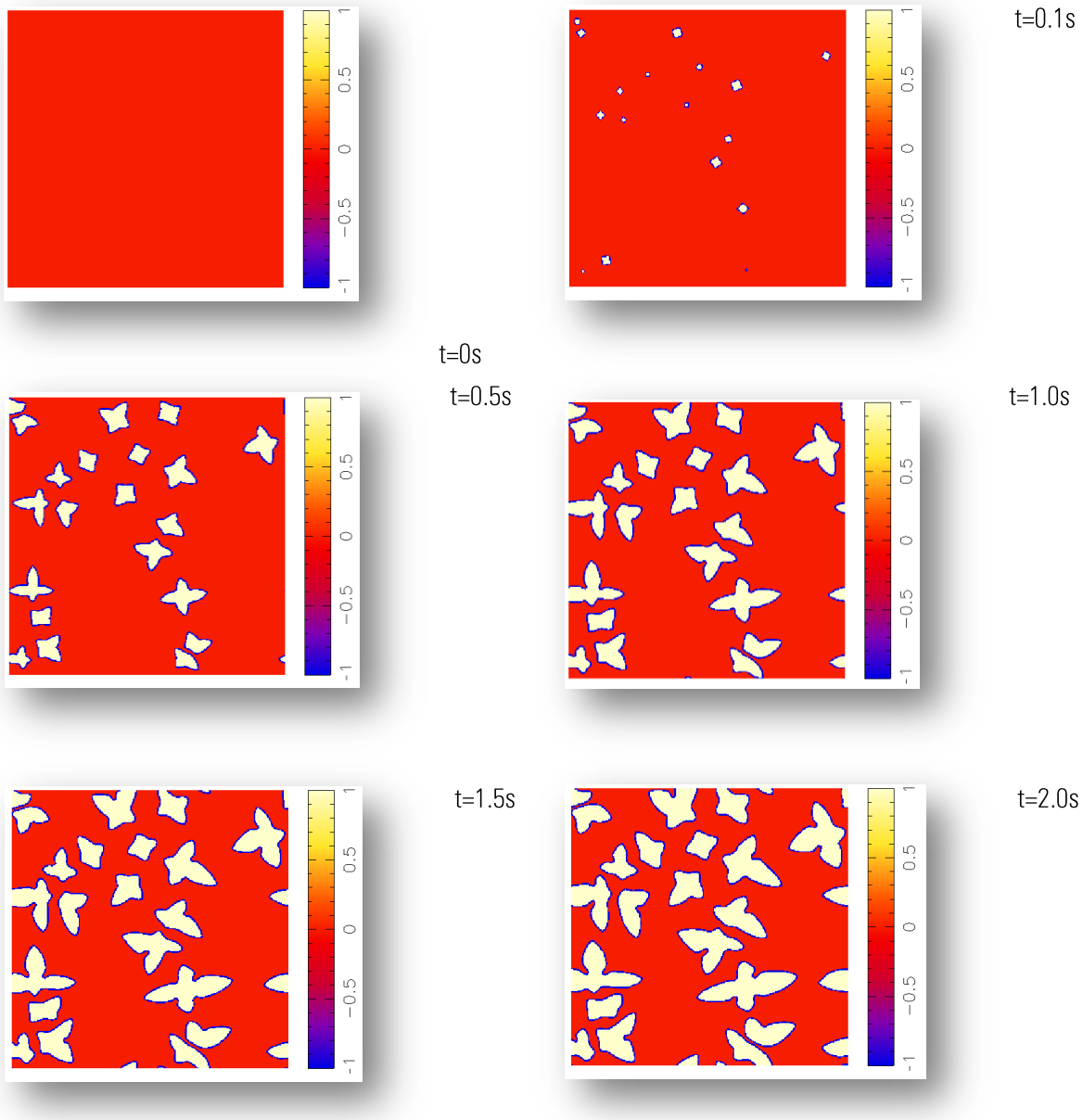
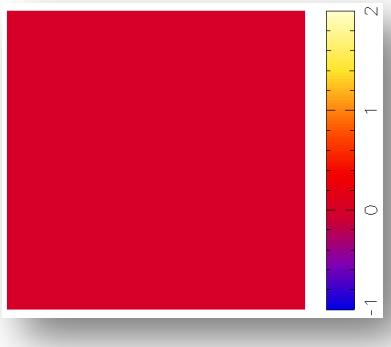


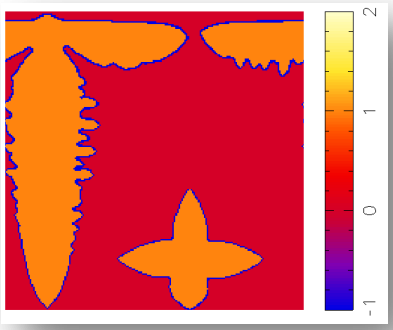
Figure 5.4. The solidification path: AlCu_Equiaxed_dri.txt.
Example: AlCu_Equiaxed_phas. .

5.3.3 AlCu_Temp1d_dri.txt

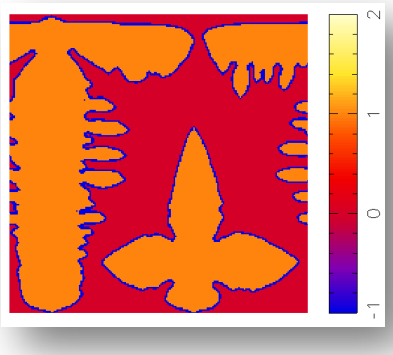
- Solidification sequence presented by the .phas-output (phase numbers: -1 ⟶ interface; 0 ⟶ liquid; 1 ⟶ fcc_A1 phase, 2 ⟶ AlCu_THETA)



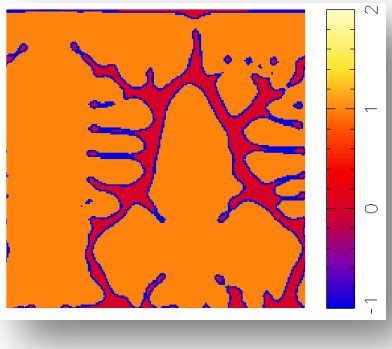
t=0s



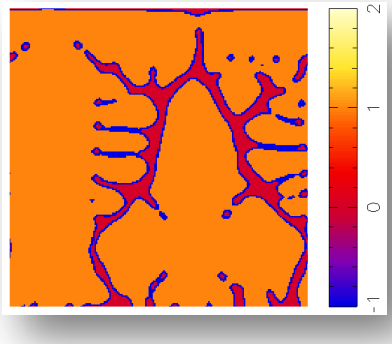
t=9.0000004Ex10^-2s



t=0.1s



t=0.3s



t=0.4s

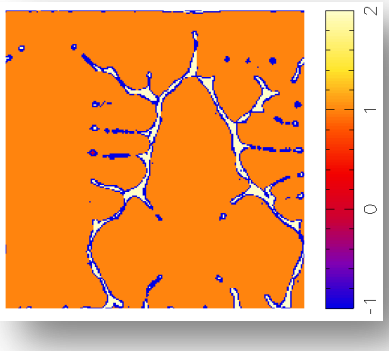


Figure 5.5. The solidification sequence for the driving file AlCu_Temp1d_dri.txt

- Concentration AlCu_Temp1d_conc1.mcr

t=0.4s

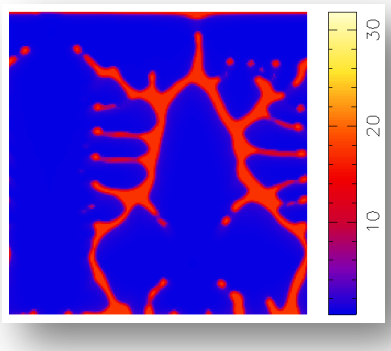


Figure 5.6. Concentration of copper after 0.4 seconds for driving file AlCu_Temp1d_dri.txt

6 "Gamma-Alpha"

6.1 Description

A series of examples ("Gamma_Alpha_dri", "Gamma_Alpha_TQ_dri" and "Gamma_Alpha_Stress_dri") simulate the $\gamma \rightarrow \alpha$ transformation for a ternary steel model alloy (iron, carbon and manganese). The first two examples are intended to demonstrate the difference between MICRESS® simulations with and without coupling to Thermo-Calc™. Both are concentration-coupled (either linearized phase diagrams OR database use) and demonstrate the use of the "seed-undercooling" nucleation model. The third example shows how stress coupling and stoichiometric phases can be included.

A variation of the "Gamma_Alpha_TQ_dri"-model, the "GammaAlphaCementite_LinTQ_dri", demonstrates the application of a combination between linearized phase diagrams AND coupling to a thermodynamic database. Another variation of the "Gamma_Alpha_TQ_dri"-example, "GammaAlphaCementiteTQ_dri", utilizes only coupling to a thermodynamic database. The main features of the individual models in the group "Gamma-Alpha" are reviewed in the next section. The "Gamma_Alpha_NPLE_dri" demonstrates the use of special solute partitioning options (NPLE = non-partitioning, local equilibrium) and their effect on the γ–α transformation. This example will be complemented by GammaAlpha_Para.dri, GammaAlpha_Pearlite.dri and GammaAlpha_ParaTQ.dri examples in the next release of this manual. Respective files are however already included in the MICRESS Version 6.0 distribution CD.

name dri file	Gamma_Alpha_dri.txt Gamma_Alpha_TQ_dri.txt Gamma_Alpha_Cementite_LinTQ_dri.txt Gamma_Alpha_CementiteTQ_dri.txt Gamma_Alpha_NPLE_dri.txt Gamma_Alpha_Stress_dri
alloy system	Fe-C-Mn (FeCMn.Ges5)
composition	$3.2.10^{-3}$wt% C 0.174 wt% Mn
transition	solid phase transition

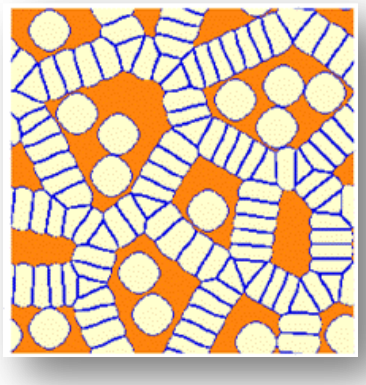


Table 6 Overview gamma-alpha examples

6.2 Simulation conditions

name dri file		Gamma_Alpha_dri.txt	Gamma_Alpha_TQ_dri.txt	Gamma_Alpha_Cementite_LinTQ_dri.txt	Gamma_Alpha_CementiteTQ_dri.txt	Gamma_Alpha_NPLE_dri.txt	Gamma_Alpha_Stress_dri
dimension		2D					3D
grid size (cells)		250x1x250					50x20x50
grid spacing		0.25µm					0.5µm
interface thickness (cells)		5					4
boundary conditions BCs							
phase field BCs	East:	periodic	periodic	periodic	periodic	periodic	periodic
	West:	periodic	periodic	periodic	periodic	periodic	periodic
	North:	---	---	---	---	---	insulation
	South:	---	---	---	---	---	insulation
	bottom	periodic	periodic	periodic	periodic	periodic	periodic
	top:	periodic	periodic	periodic	periodic	periodic	periodic
concentration field BCs	East:	periodic	periodic	periodic	periodic	periodic	periodic
	West:	periodic	periodic	periodic	periodic	periodic	periodic
	North:	---	---	---	---	---	insulation
	South:	---	---	---	---	---	insulation
	bottom:	periodic	periodic	periodic	periodic	periodic	periodic
	top:	periodic	periodic	periodic	periodic	periodic	periodic
solid phases:		2 solid phases: γ, α		3 solid phases: γ, α, cementite		2 solid phases: γ, α	3 solid phases: γ, α, cementite
grain input		deterministic					random: integer for randomization: 7
		placement of 9 grains of α-phase (round)					12 grains of one type of grains (round)
		stabilisation of the grains); Voronoi construction					
		further nucleation: enabled					
		seed types:3		seed types:5		seed types:3	

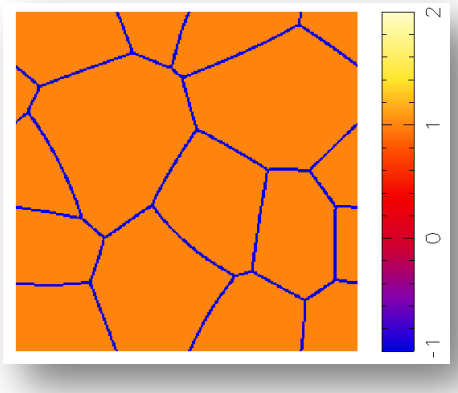
<table>
<tr><td></td><td colspan="4">seed positions: triple, interface, bulk</td><td>seed positions: triple, interface</td></tr>
<tr><td></td><td colspan="4">seed undercooling nucleation model applied</td><td></td></tr>
<tr><td></td><td colspan="5">simultaneous nucleation: automatic</td></tr>
<tr><td></td><td colspan="2">temperature conditions: T_0=1100 K; G = 0 K/cm; dT/dt = -10 K/s</td><td>temperature conditions: T_0=1030 K; G = 0 K/cm; dT/dt = -10 K/s</td><td>temperature conditions: T_0=1070 K; G = 0 K/cm; dT/dt = -10 K/s</td><td>temperature conditions: T_0=1095 K; G = 0 K/cm</td></tr>
<tr><td></td><td colspan="5">latent heat: NO</td></tr>
<tr><td>output</td><td colspan="5">files: restart, grains, phases, average fraction table, interface, driving force, grain time, concentration, reference phase concentration, monitoring outputs</td></tr>
<tr><td></td><td colspan="4"></td><td>normal stress, von Mieses stress output, displacement data</td></tr>
<tr><td></td><td colspan="2">times:
output at 00.25 and 01.00 s
from 01.00 s to 10 s output every 0.5 s (linear step)
from 10.00 s to 25 s output every 1 s (linear step)</td><td>times:
output at 00.25 and 01.00 s
from 01.00 s to 10 s output every 0.5 s (linear step)
from 10.00 s to 35 s output every 1 s (linear step)</td><td>times:
output at 00.25 and 01.00 s
from 01.00 s to 10 s output every 0.5 s (linear step)
from 10.00 s to 25 s output every 1 s (linear step)</td><td>times:
output at 5, 10 and 15 s</td></tr>
<tr><td>special features</td><td colspan="4">concentration coupling</td><td>concentration and stress coupling</td></tr>
<tr><td></td><td colspan="4">NO 1d far field diffusion approximation</td><td></td></tr>
<tr><td></td><td rowspan="3">no thermo-dynamic coupling</td><td colspan="3">thermodynamic coupling: enabled</td><td rowspan="3">no thermo-dynamic coupling</td></tr>
<tr><td>Steel.Ges5</td><td colspan="2">FECMn.Ges5</td></tr>
<tr><td>database global</td><td>linearTQ</td><td>database global</td></tr>
<tr><td></td><td colspan="5">NO moving frame</td></tr>
</table>

Table 7 GammaAlpha Examples: Overview of simulation conditions/ parameters

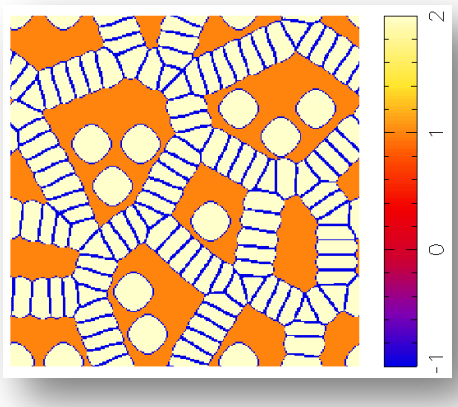
6.3 Visualisation of the results

6.3.1 GammaAlpha_dri and GammaAlpha_TQdri

Gamma_Alpha_TQ_in.txt. Example: Gamma_Alpha_TQ_phas.mcr

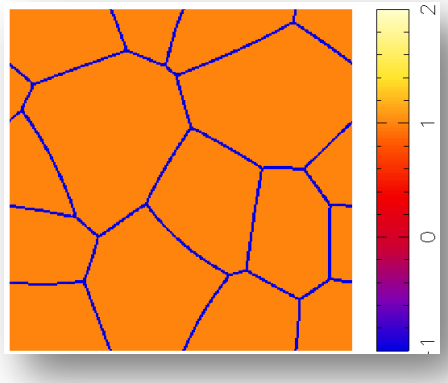


t=0s

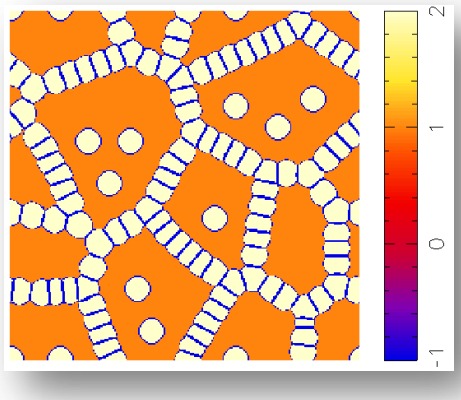


t=25s

Gamma_Alpha_in.txt Example: Gamma_Alpha_phas.mcr



t=0s

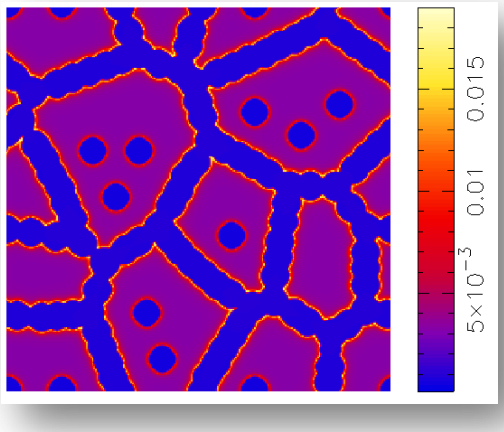


t=25s

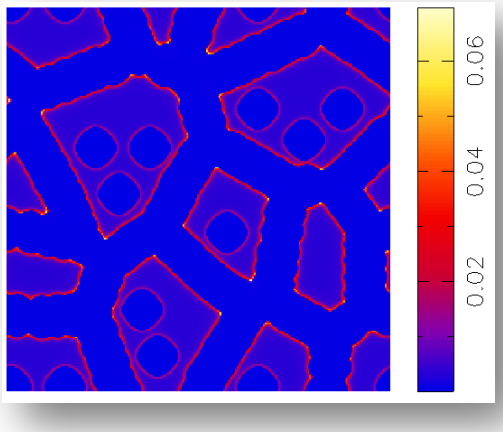
Figure 6.1. The phase transition sequence for the driving files: Gamma_Alpha_in.txt and Gamma_Alpha_TQ_in.txt

- Concentration output for t=25s

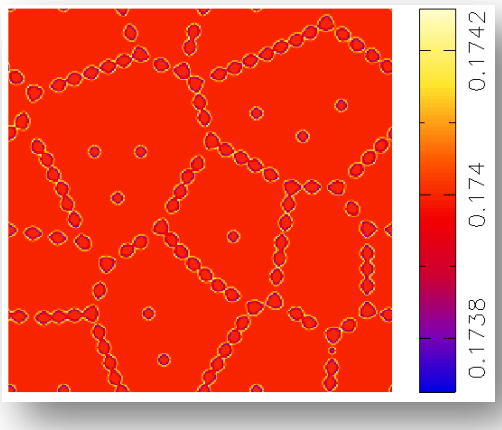
Gamma_Alpha_in.txt: Carbon concentration. Example: Gamma_Alpha_conc1.mcr



Gamma_Alpha_TQ_in.txt: Carbon concentration. Example: Gamma_Alpha_TQ_conc1.mcr



Gamma_Alpha_in.txt: Manganese concentration. Example: Gamma_Alpha_conc2.mcr



Gamma_Alpha_TQ_in.txt: Manganese concentration. Example: Gamma_Alpha_TQ_conc2.mcr

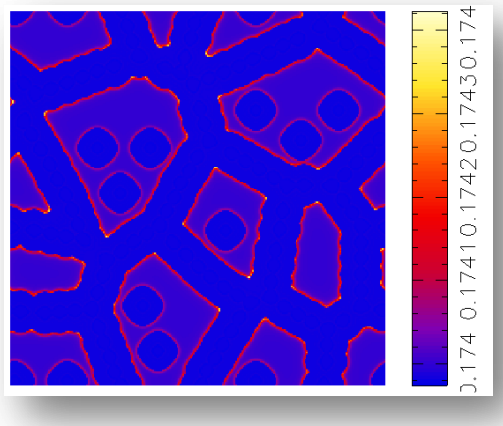


Figure 6.2. Concentration: "Gamma-Alpha" with (right) and without (left) TQ-coupling

6.3.2 GammaAlpha_Cementite_LinTQ_dri and _Cementite_TQ_dri

Phase transition path presented by the .phas-output. **Note**: Same results, but different colour codes used for the output! (-1 –interface; 0 –not assigned , 1 –gamma; 2 –alpha; 3 –cementite)

Gamma_Alpha_Cementite_LinTQ_phas.mcr	Gamma_Alpha_Cementite_TQ_phas.mcr
t=0s	t=0s
t=6.5s	t=8s
t=13s	t=20s
t=35s	ljt=35s

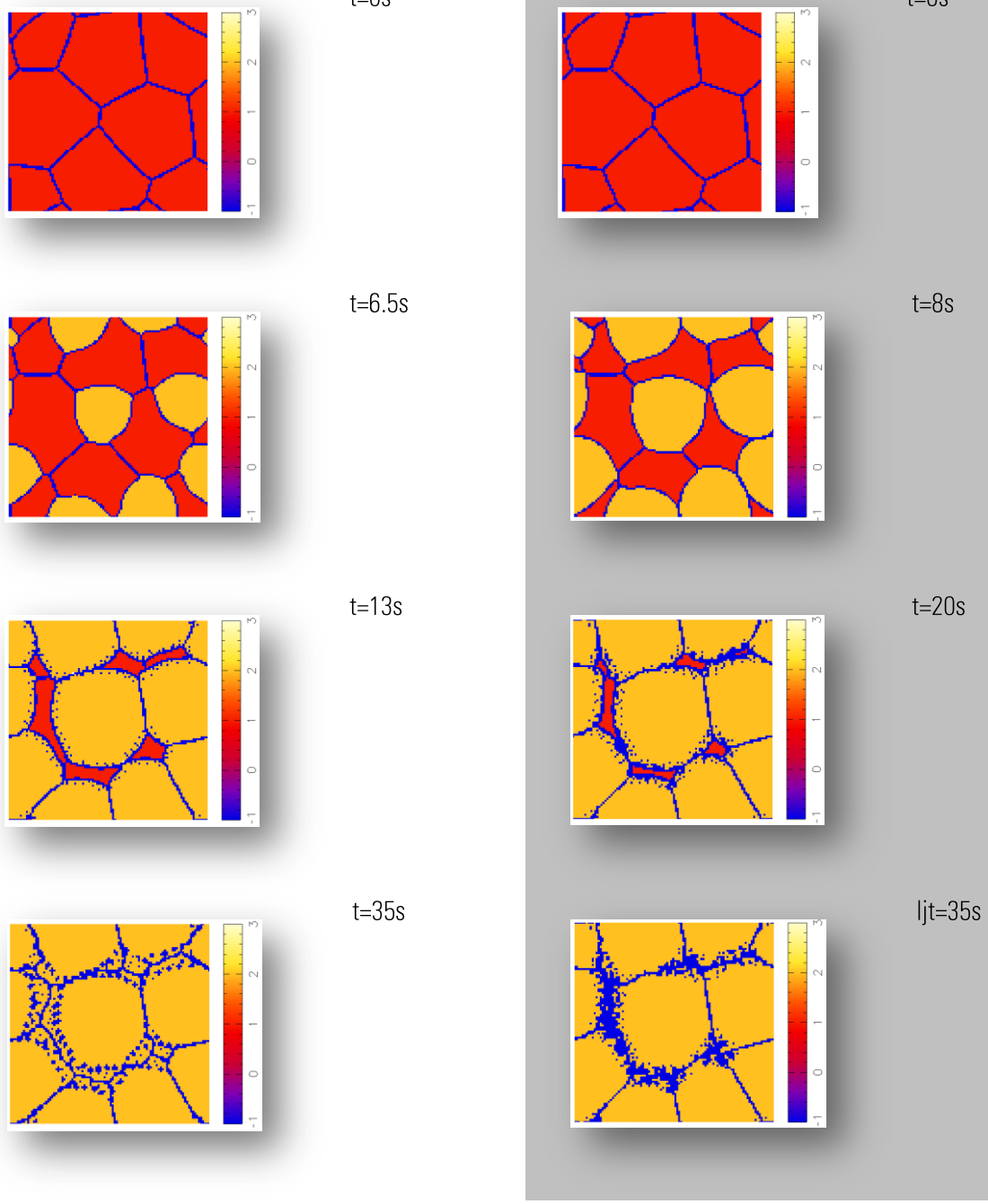


Figure 6.3. The phase transition path: GammaAlpha_Cementite_LinTQ_dri and GammaAlpha_CementiteTq_dri

- Concentration

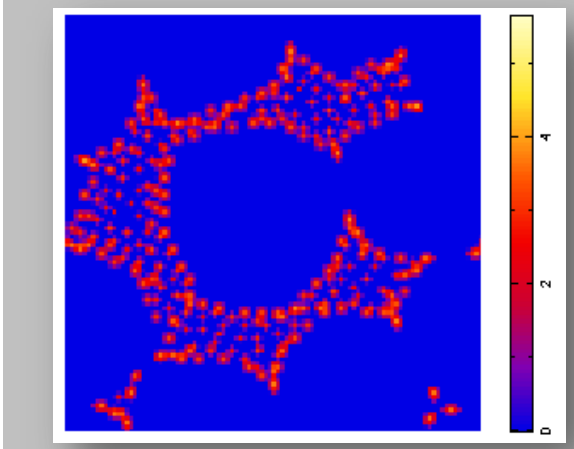
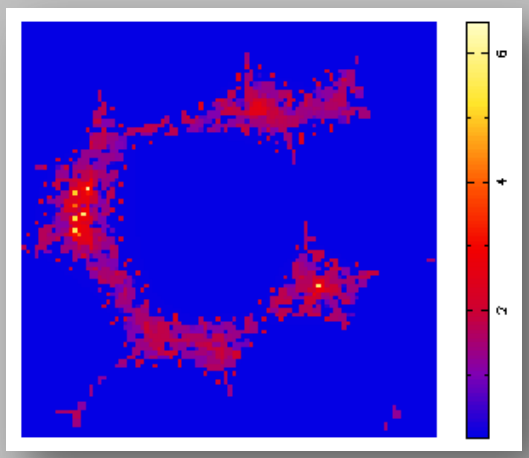
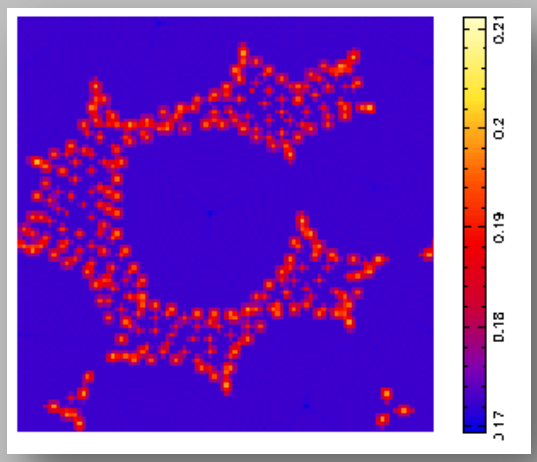
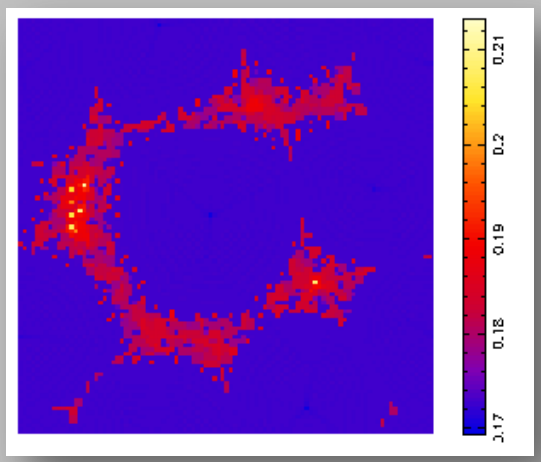
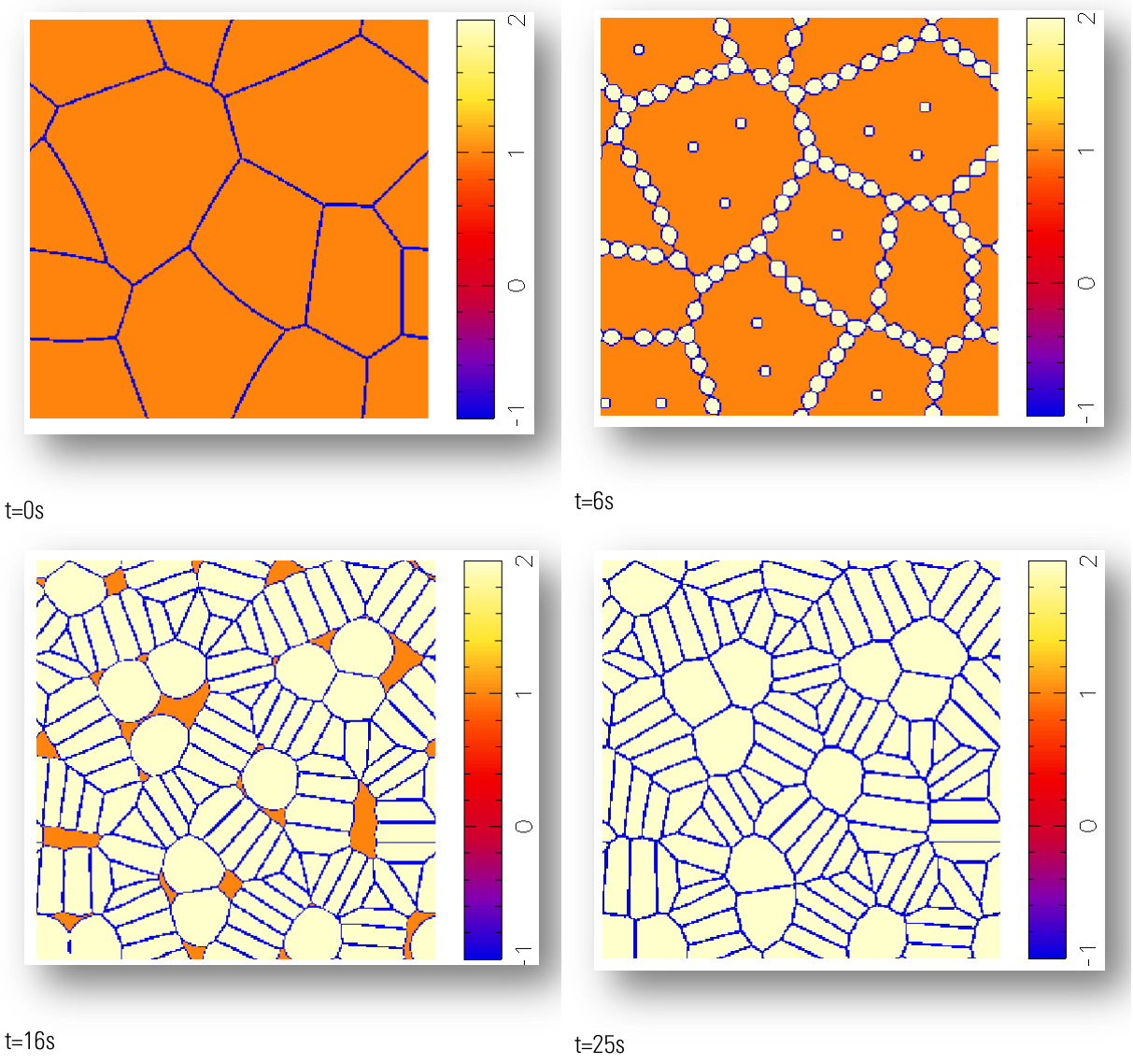
Gamma_Alpha_Cementite_LinTQ_in.txt, Carbon Concentration	Gamma_Alpha_CementiteTQ_in.txt, Carbon Concentration
	
Gamma_Alpha_Cementite_LinTQ_in.txt, Manganese concentration	Gamma_Alpha_CementiteTQ_in.txt, Manganese concentration
	

Figure 6.4. Concentration: "Gamma-Alpha_Cementite" with linearized (LinTQ) and non-linearised (TQ) concentration-coupling (time step 35 sec in both cases)

6.3.3 Gamma_Alpha_NPLE_dri

Solidification path presented by the .phas-output (-1 –interface; 0 –not assigned , 1 –gamma; 2 –alpha)



t=0s t=6s

t=16s t=25s

Figure 6.5. The phase transition sequence for Gamma_Alpha_NPLE_in.txt

- Concentration fields

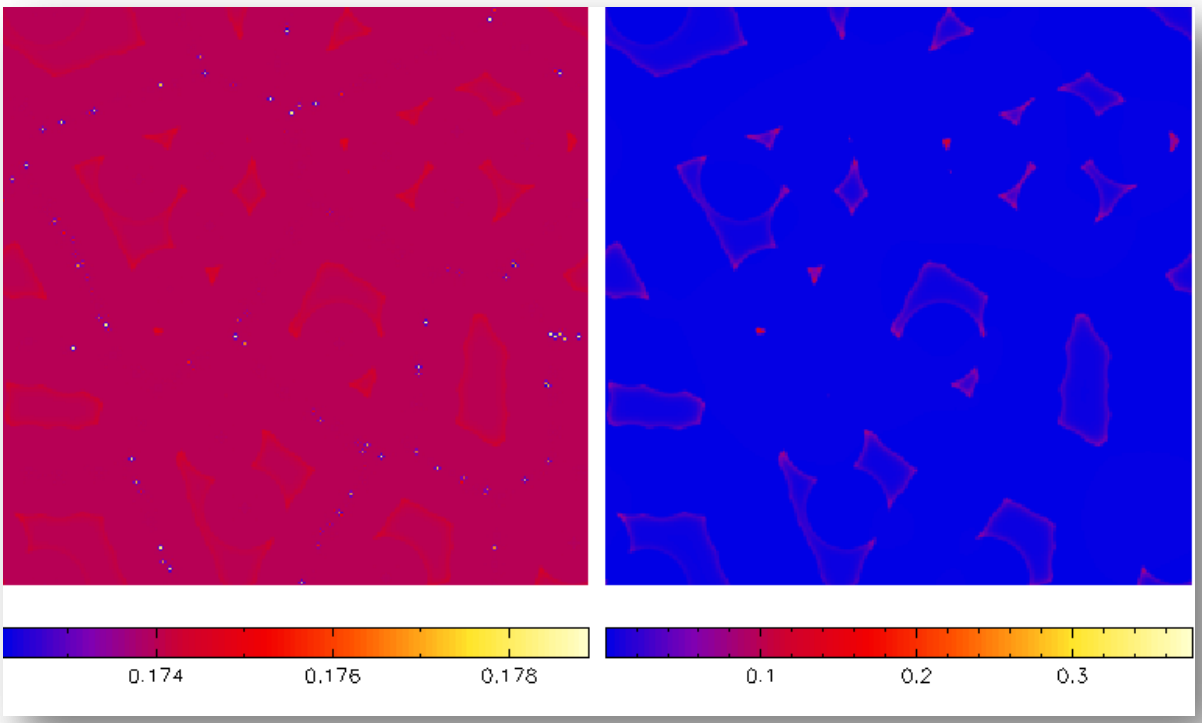
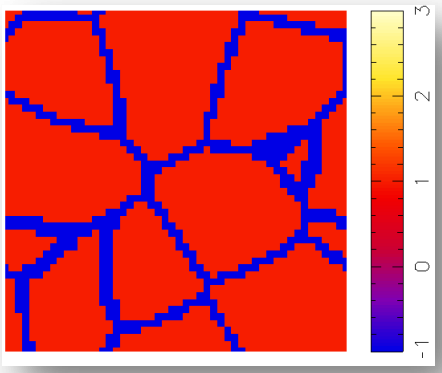


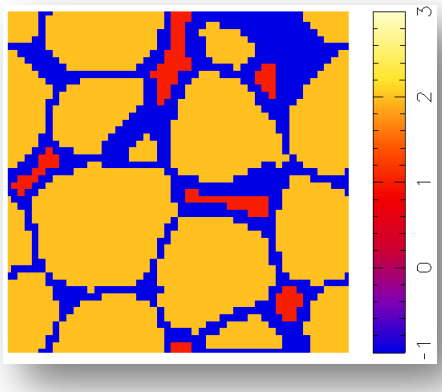
Figure 6.6: Concentration fields for Mn (left) and C (right) for the Gamma-Alpha_NPLE example at t=15 sec

6.3.4 Gamma_Alpha_Stress_dri

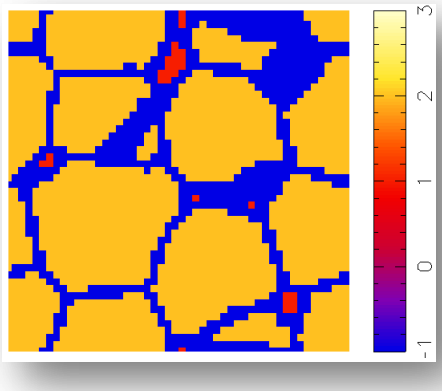
- Transformation sequence presented by the .phas-output (-1 –interface; 0 –not assigned , 1 –gamma; 2 –alpha; 3 –cementite)



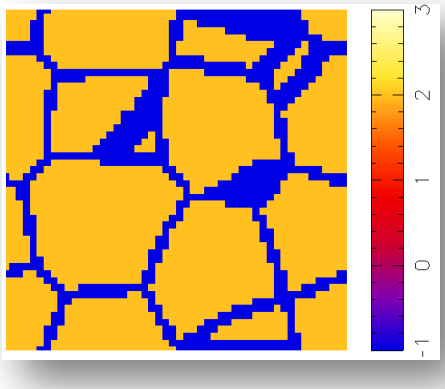
t=0s



t=6s



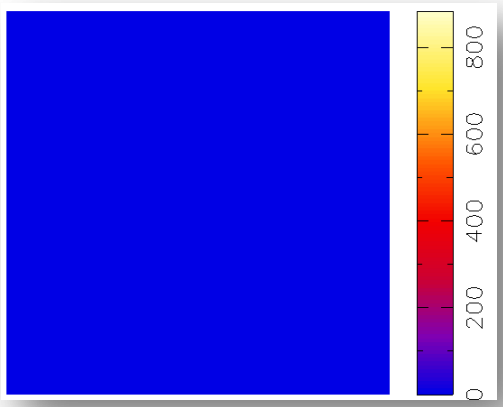
t=10s



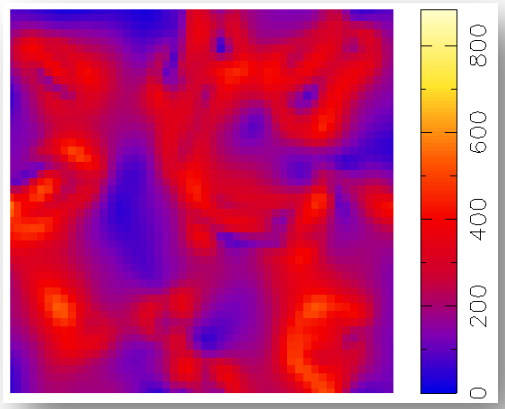
t=15s

Figure 1. The phase transition sequence: Gamma_Alpha_Stress_in.txt

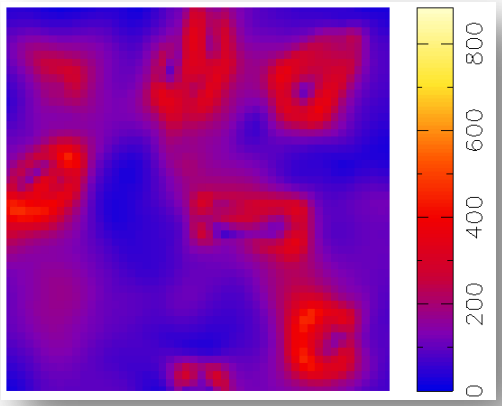
- Von Mises stress



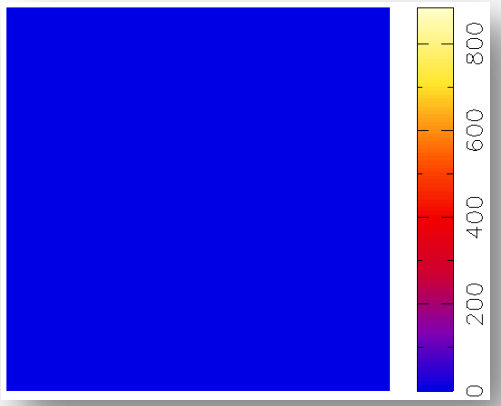
t=0s



t=5s



t=10s



t=15s

Figure 6.8. Equivalent stresses for the "Gamma-Alpha_Stress" example

7 "Grain-Growth"

7.1 Description

The group of examples "Grain Growth" ("Grain_Growth_dri", "Grain_Growth_Particle_Pinning_dri" and "Grain_Growth_Solute_Drag_dri" shows how MICRESS® can be used without coupling to external fields like temperature or concentration, i.e. using only the curvature as a driving force for the transformation. Respective curvature based coarsening is inherent to phase-field models. These examples show how to read-in initial microstructures. The "Grain_Growth_dri" example displays "pure" grain growth, whereas the other examples draw on specific models hindering grain boundary motion like e.g. the particle-pinning, the solute-drag and KTH-solute-drag models, respectively

In addition, grain growth with non-linear temperature profiles is modeled in the „Grain_Growth_Profiles_dri" example. The example "Grain_Growth_Solute_Drag_dG_in.txt" is the same as "Grain_Growth_Solute_Drag_in.txt" apart from the mobility which is not constant but dependent on the driving force.

name dri file	Grain_Growth_in.txt Grain_Growth_Particle_Pinning_in.txt Grain_Growth_Profiles_in.txt Grain_Growth_Solute_Drag_dG_in.txt Grain_Growth_Solute_Drag_in.txt
alloy system	not specified e.g. steel
composition	not specified e.g. austenite
modelled phenomenon	grain growth with/without pinning

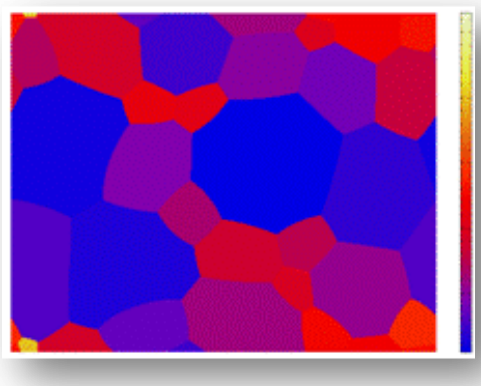


Table 8 Examples: Grain-Growth details

7.2 Simulation conditions

name dri file		Grain_Growth_in.txt	Grain_Growth_Particle_Pinning_in.txt	Grain_Growth_Solute_Drag_in.txt	Grain_Growth_Solute_Drag_dG_in.txt	Grain_Growth_Profiles_in.txt
dimension		2D				
grid size (cells)		400x1x320				100x1x500
grid spacing		1.5µm				
interface thickness (cells)		5				
boundary conditions BCs						
phase field BCs	East:	periodic	periodic	periodic	periodic	periodic
	West:	periodic	periodic	periodic	periodic	periodic
	bottom	periodic	periodic	periodic	periodic	periodic
	top:	periodic	periodic	periodic	periodic	periodic
solid phases:		1 solid phases				
grain input		from file: Grain_Growth_Microstructure.txt				random : integer randomization: 123; 100 different round grains with stabilisation and voronoi construction
		further nucleation: NO				
		phase interaction: pure	phase interaction: with particle pinning	phase interaction: with solute drag	phase interaction: pure	
		mobility: constant			mobility: dg_dependent Grain_Growth_dG_Mobility_Data	mobility: temperature dependent
		temperature conditions: T_0=1000 K; G = 0 K/cm; dT/dt = 0 K/s (isothermal)				from file

output	files: restart, grains, phases, interface, mobility, curvature, velocity, grain-time file, von Neumann Mullins output, monitoring outputs				
	times: from 0.00 s to 20 s output every 5 s (linear step) from 20.00 s to 250 s output every 10 s (linear step) from 250.00 s to 1000 s output every 50 s (linear step)				times: from 0.00 s to 0.4 s output every 0.02 s (linear step) from 0.4 s to 1 s output every 0.05 s (linear step)
special features	phase field coupling				
	no thermodynamic coupling				
	microstructure read in from file Grain_Growth_Microstructure.txt				
	NO moving frame				
				driving force dependent mobility	temperature dependent mobility -> temperature trend read in from file

Table 9 Example: Grain Growth: field parameters

7.3 Visualisation of the results

7.3.1 Pure grain growth and grain growth with particle pinning and solute drag

- Grain growth sequence presented by the .korn-output (each grain has a different colour)

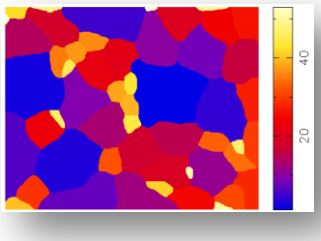
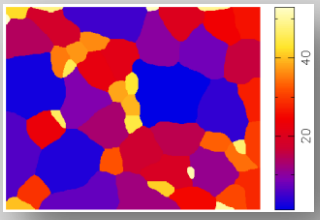
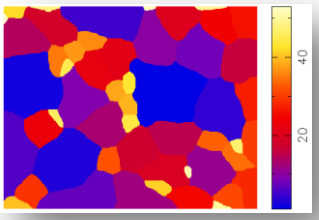
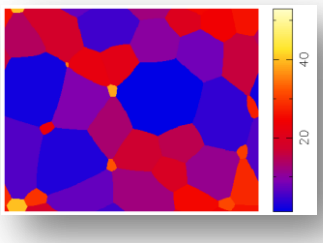
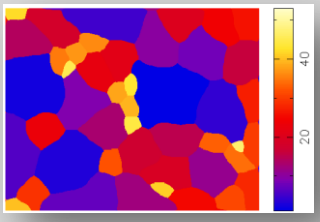
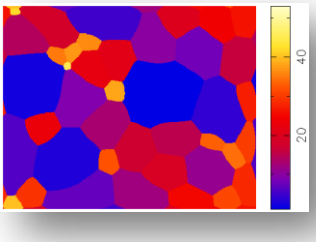
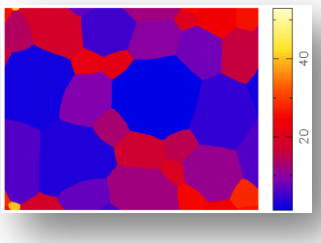
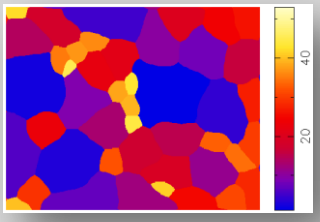
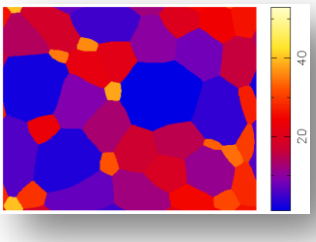
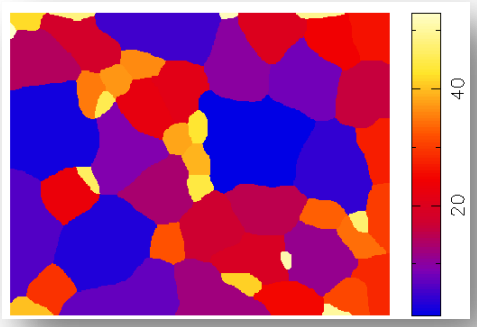
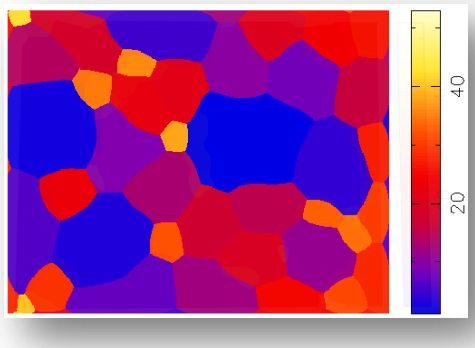
Grain_Growth_in.txt	**Grain_Growth_Particle_Pinning_in.txt**	**Grain_Growth_Solute_Drag_in.txt**
		
t=0s	t=0s	t=0s
		
t=500s	t=500s	t=500s
		
t=1000s	t=1000s	t=1000s

Figure 7.1. Grain growth sequence presented by the .korn-output (each grain has a different colour)

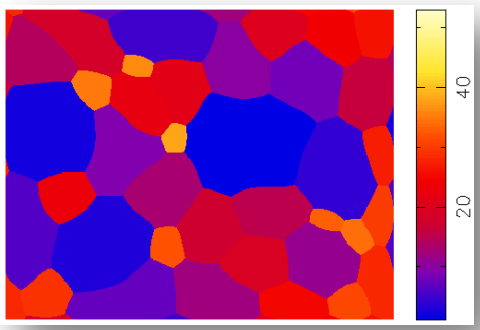
7.3.2 Grain_Growth_Solute_Drag_dG_in.txt



t=0s



t=500s

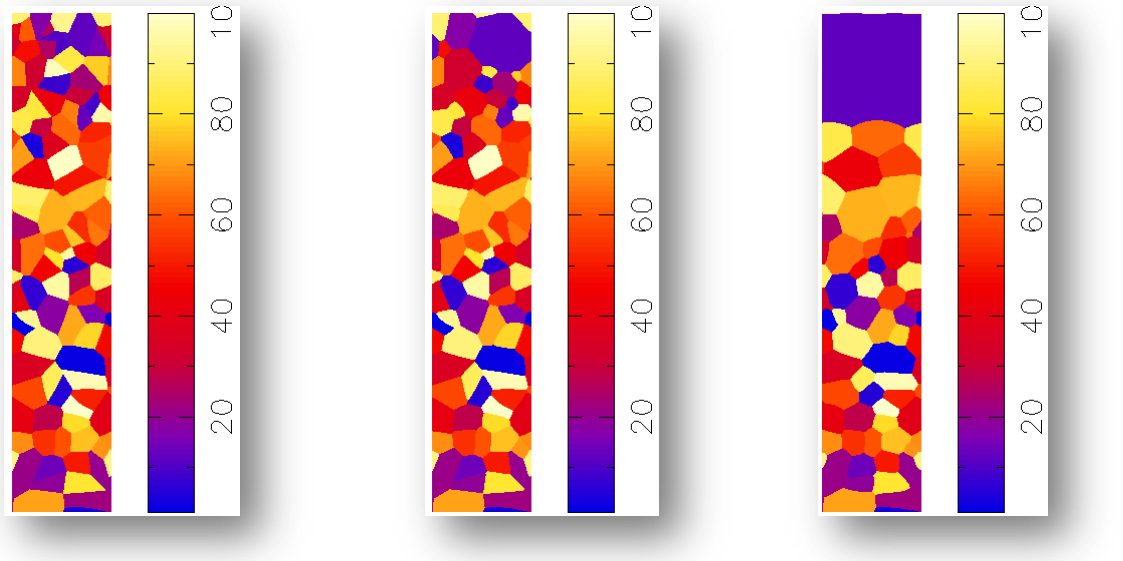


t=1000s

Figure 2. The grain growth sequence with driving force dependent mobility (Grain_Growth_Solute_Drag_dG_korn.txt)

7.3.3 Grain_Growth_Profiles_in.txt

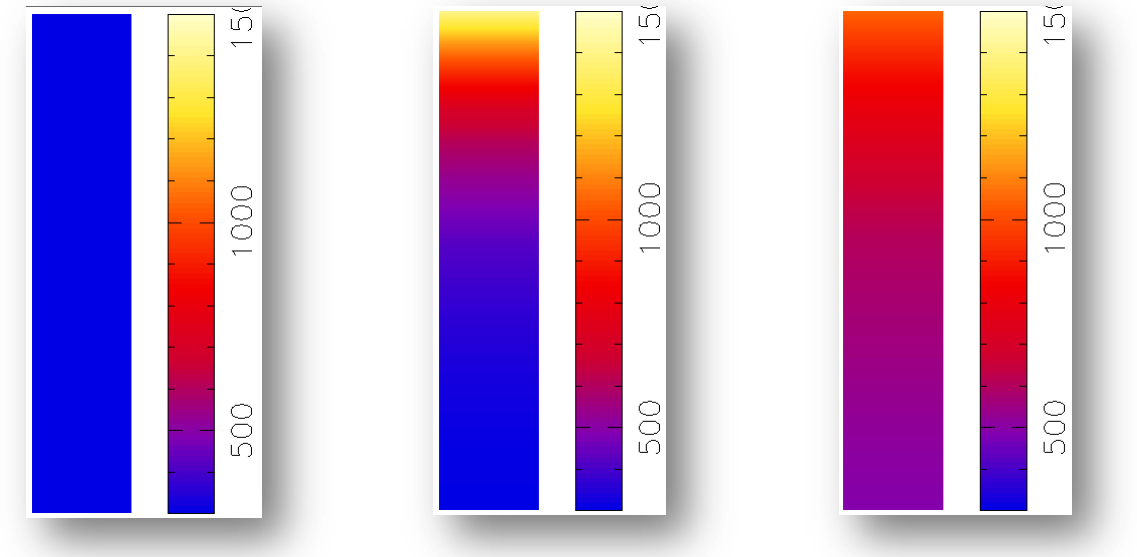
- Grain growth: Grain_Growth_Profiles_korn.txt



t=0s t=0.32s t=1s

Figure 3. The grain growth path with temperature dependent mobility

- Temperature distribution: Grain_Growth_Profiles_temp.txt



t=0s t=0.32s t=1s

Figure 4. The temperature profiles for different time steps

8 "Phosphorous Peak"

8.1 Description

These two examples, "P_Peak_1D_dri" and "P_Peak_2D_dri" show full multicomponent diffusion with coupling to Thermo-Calc™ using industrial steel grades. The first example is one-dimensional and provides a ready benchmark against DICTRA™.

name dri file	P_Peak_1D_in.txt P_Peak_2D_in.txt
alloy system	Fe-C-Mn-Si-P (Fe_C_Mn_Si_P.Ges5)
composition	0.4 wt% C 0.8 wt% Mn 0.7 wt% Si 3.10^{-2} wt% P
transition	solidification

Table 10 Example: Phosphorous Peak details: modelled phases are liquid(red), ferrite(orange) and austenite (bright)

8.2 Simulation conditions

name dri file		P_Peak_1D_in.txt	P_Peak_2D_in.txt
dimension		1D	2D
grid size (cells)		1x1x200	400x1x400
grid spacing		0.5µm	2µm
interface thickness (cells)		5	4
boundary conditions BCs			
phase field BCs	east: west: bottom top:	insulation insulation insulation insulation	symmetric symmetric periodic periodic
concentration field BCs	east: west: bottom: top:	insulation insulation insulation insulation	periodic periodic periodic periodic
solid phases:		2 solid phases: BCC_A2 (ferrite), FCC_A1 (austenite)	
grain input		deterministic placement of 1 grain (round, coordinates: x=0.25, z=0.25, r=0), stabilisation of the grains); no voronoi construction	
		rotation angle 0°	rotation angle 45°
		Max. number of new nuclei: 1	Max.number of new nuclei: 250
		further nucleation: enabled	
		seed types:1, seed position: interface	
			simultaneous nucleations: automatic
temperature		temperature conditions: T_0=1763.75 K; G = 0 K/cm; dT/dt = -0.2 K/s	
		latent heat: NO	

output	files: restart, grains, phases, average fraction table, concentration, concentration of the reference phase, average concentration per phase, linearization output, monitoring outputs	
	times: from 00.00 s to 700 s output every 50 s (linear step) from 700 s to 2500 s output every 100 s (linear step)	times: from 00.00 s to 160 s output every 10 s (linear step) from 160 s to 170 s output every 2.5 s (linear step) from 170 s to 200 s output every 10 s (linear step) from 200 s to 600 s output every 50 s (linear step) from 600 s to 3000 s output every 100 s (linear step)
special features	concentration coupling	
	NO 1d far field diffusion approximation	
	thermodynamic coupling: enabled; Fe_C_Mn_Si_P.Ges5 datafile	
	NO moving frame	

Table 11 Example: Phosphorus Peak: field parameters

8.3 Visualisation of the results

8.3.1 P_Peak_1D_in.txt

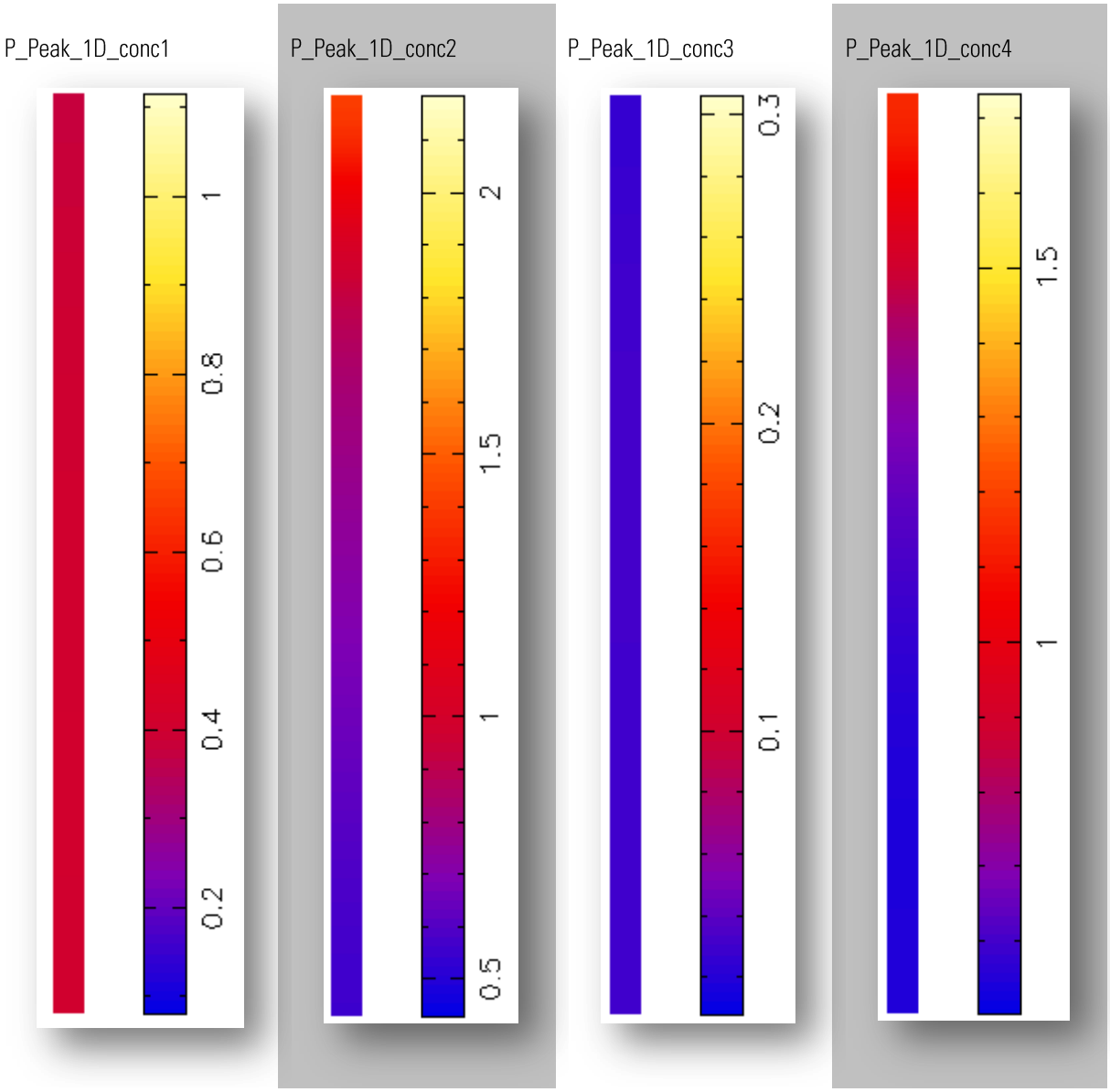


Figure 5. The 1D concentration field: P_Peak_1D_conc1.mcr to P_Peak_1D_conc4.mcr (1:C, 2:Mn, 3:P and 4: Si) for t=2000s.

8.3.2 P_Peak_2D_in.txt

- Solidification sequence presented by the .phas-output (-1 ⟶ interface; 0 ⟶liquid , 1 ⟶ BCC_A2 (ferrite), 2 ⟶ FCC_A1 (austenite))

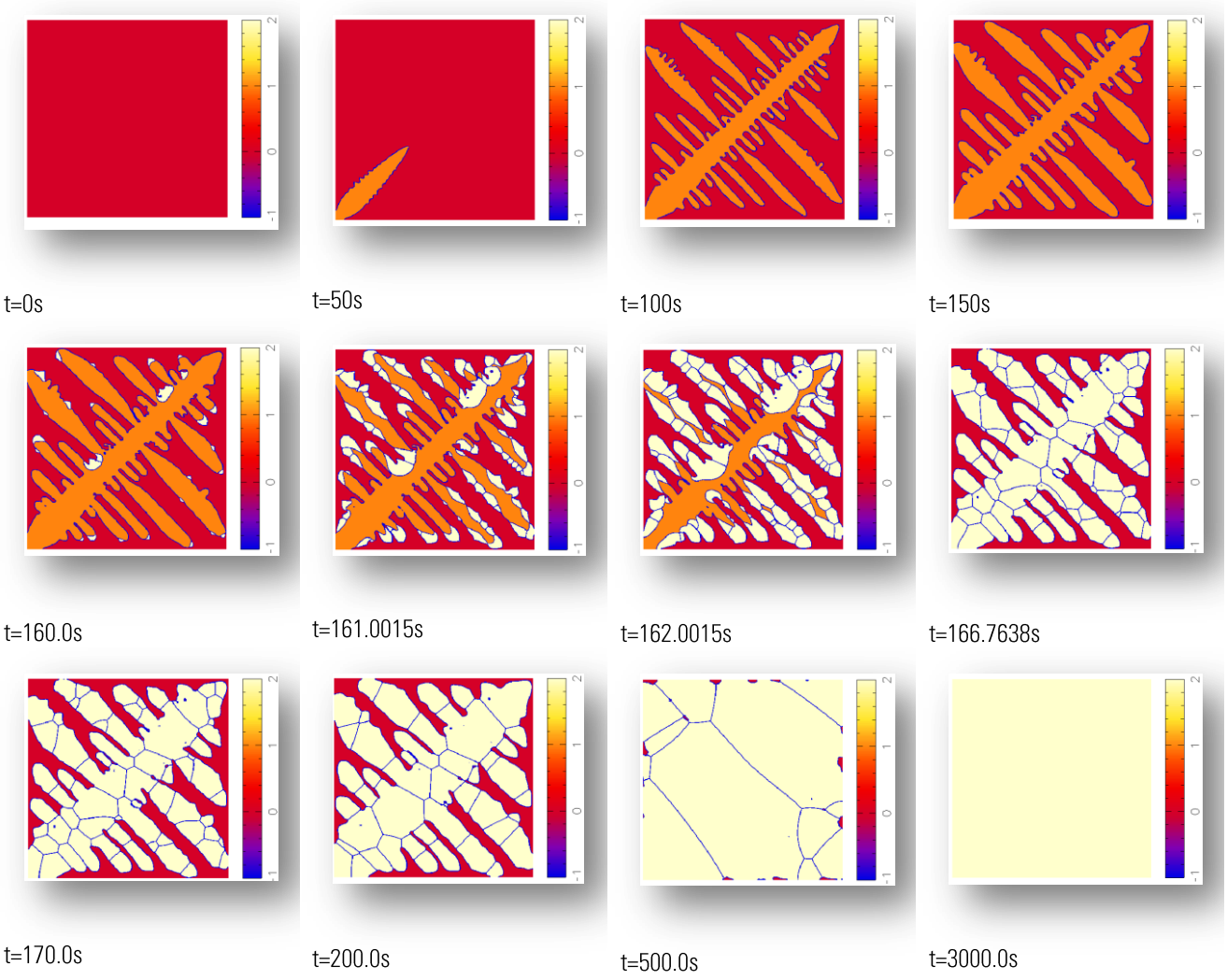
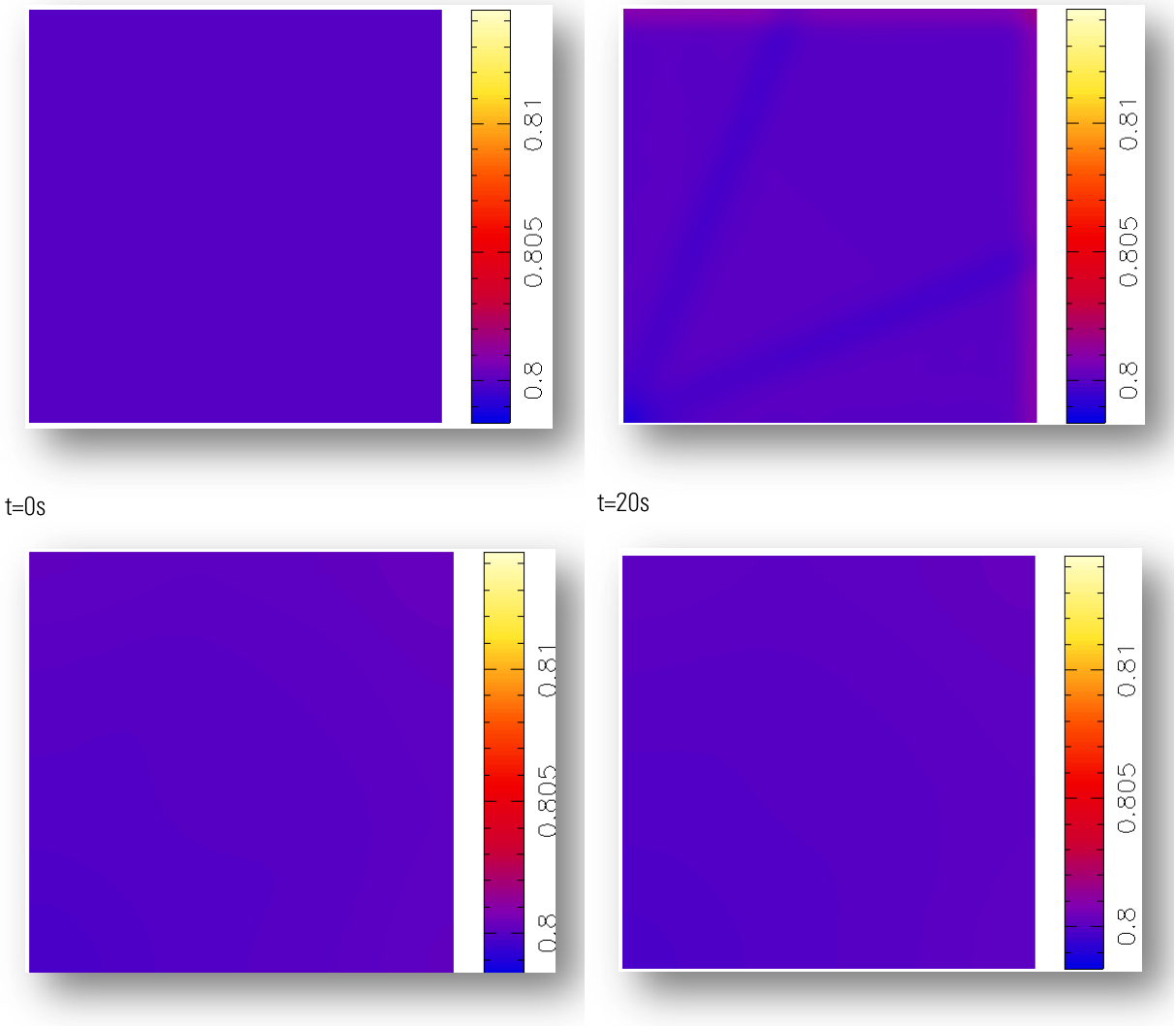


Figure 6. The solidification path: P_Peak_2D_phas.mcr

- *Concentration evolution presented for the .conc2 (Mn)*



t=0s t=20s

t=700s t=1000s

Figure 8.3. The concentration field for Manganese: P_Peak_2D_conc2.mcr (Mn) (1: C, 2: Mn, 3: P and 4: Si)

9 "Recrystallisation"

9.1 Description

The five examples, "ReX_1_dri", "ReX_2_dri", "ReX_3_dri", "ReX_4_dri", and "ReX_5_dri" illustrate various topics related to recrystallisation. All examples show the influence of misorientation and stored-energy on recrystallisation/growth and the use of the Voronoi criterion. In addition, "ReX_1_dri" and "ReX_5_dri" demonstrate the use of the "seed-undercooling" nucleation model.

name dri file	ReX_1_in.txt ReX_2_in.txt ReX_3_in.txt ReX_4_in.txt ReX_5_in.txt
alloy system	Not specified: e.g. steel
composition	Not specified: e.g. ferrite or austenite
phenomenon	recrystallisation

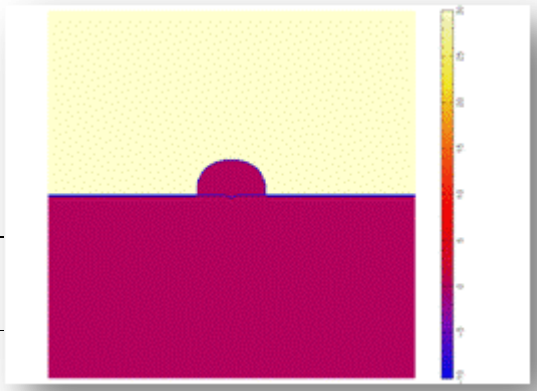


Table 12 Example Recrystallisation: details

9.2 Simulation conditions

name dri file		ReX_1_in.txt	ReX_2_in.txt	ReX_3_in.txt	ReX_4_in.txt	ReX_5_in.txt
dimension		2D				
grid size (cells)		400x1x400	500x1x500	400x1x400	500x1x300	500x1x1000
grid spacing		0.25µm	0.5µm	2E-02µm	0.5µm	
interface thickness (cells)		5		4	5	
boundary conditions BCs						
phase field BCs	east:	insulation	insulation	periodic	insulation	periodic
	west:	insulation	insulation	periodic	insulation	periodic
	bottom	insulation	insulation	insulation	insulation	insulation
	top:	insulation	insulation	insulation	insulation	insulation
solid phases:		1 solid phase: different stored energy assigned to different grains				
grain input		deterministic		random: integer for randomization: 13	deterministic	random: integer for randomization: 6
		3 new grains (round)	6 new grains (round)	two types of grains (type 1: 100, type 2: 30)	22 new grains (elliptic)	4 types of grains (type 1: 5, type 2: 5, type 3: 15, type 4: 5); elliptic
		stabilisation				
		Voronoi construction				
		further nucleation: NO	further nucleation: YES	further nucleation: NO	further nucleation: YES	further nucleation: YES
		phase interaction:pure mobility: constant				
		recrystallisation: phase 1: anisotropic cubic symmetry				
			misorientation			
			3 types of seeds; position of the seeds: interface, triple, bulk; seed undercooling nucleation model applied; maximum number of		2 types of seeds; position of the seeds: interface, region; seed undercooling nucleation model applied; maximum number of	2 types of seeds; seed position: interface, region; stabilisation; maximum number of simultaneous nucleations: 5

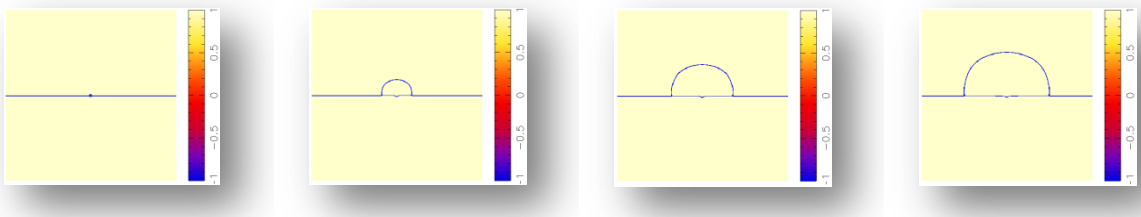
		simultaneous nucleations: 10		simultaneous nucleations: 25	
	temperature conditions: T_0=1000 K; G = 0 K/cm; dT/dt = 0 K/s			temperature conditions: T_0=1000 K; G = 0 K/cm; dT/dt = -1 K/s	
	latent heat: NO				
output	files: phases, interface, recrystallisation, recrystallized fraction output, orientation		files: orientation	files: grain number output	files: recrystallisation, miller indices, orientation
	linear step output; output at 0.2 and 2.2 s		linear step output; output at 0.05 and 0.6 s	output from 0 to 10s every 0.5 s output from 10 s to 15 s every 1 s output from 10 s to 30 s every 5 s output from 20 to 270 s every 30 s (linear step)	output from 0 to 5s every 0.5 s output from 5 s to 10 s every 1 s output from 10 s to 20 s every 2 s output from 20 to 30 s every 50 s (linear step)
special features	phase field coupling				
	no thermodynamic coupling				
	NO moving frame				

Table 13 Example: Recrystallisation: simulation conditions

9.3.1 Visualisation of the results

9.3.1 ReX_1_in.txt

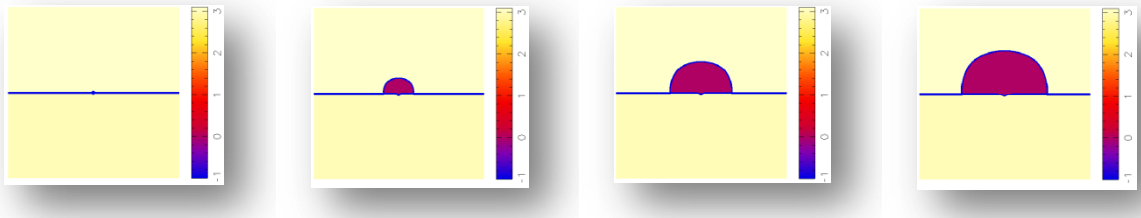
- Recrystallisation path presented by the .phas-output (-1 ⟶ interface; 0 ⟶ not assigned, 1 ⟶solid)



t=0s t=0.8s t=1.6s t=2.2s

Figure 9.1. The recrystallisation sequence: Rex_1_phas.mcr. As recrystallized grains are of the same phase, they can not be distinguished in the .phas-output. Only interfaces are visible.

- Recrystallisation path presented by the .rex-output (-1 ⟶ interface; 0: new structure/recrystallized grains , 1 ⟶ not assigned, 2 ⟶ not assigned; 3 ⟶initial structure/non-recrystallized grains)



t=0s t=0.8s t=1.6s t=2.2s

Figure 9.2. The recrystallisation sequence: Rex_1_rex.mcr. As recrystallized grains are of the same phase, they can best be distinguished in the .rex-output.

- **ReX_2_in.txt**

- Recrystallisation path presented by the .rex-output

(-1 → interface; 0: new grains, 1 → not assigned, 2 → not assigned; 3 →initial grains)

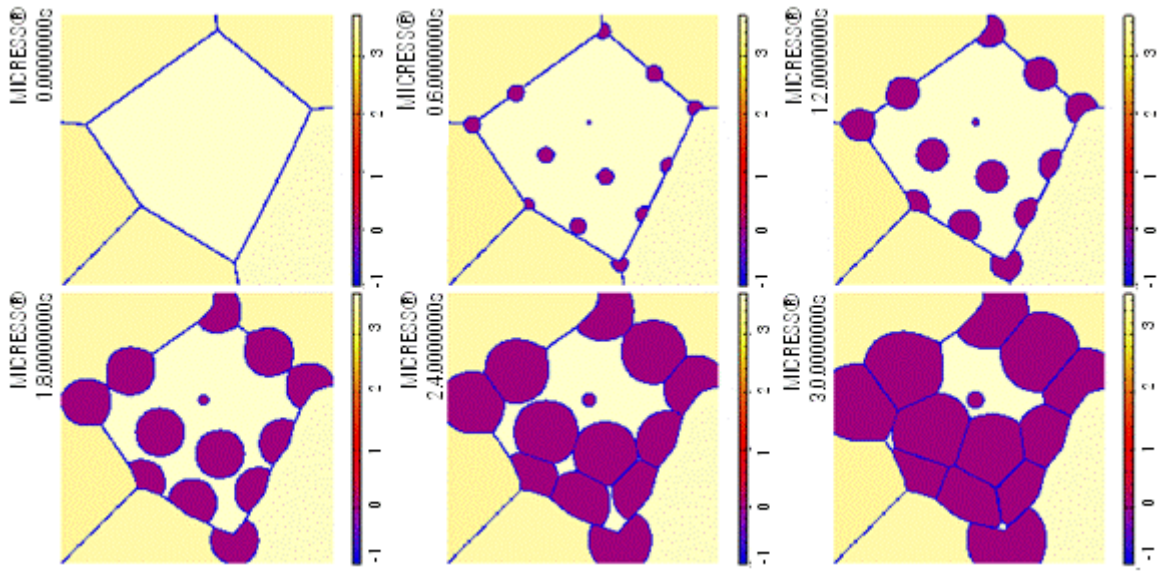


Figure 9.3: The recrystallisation sequence: Rex_2_phas.mcr

9.3.3. ReX_3_in.txt

- Recrystallisation sequence presented by the .orie-output (grain orientations)

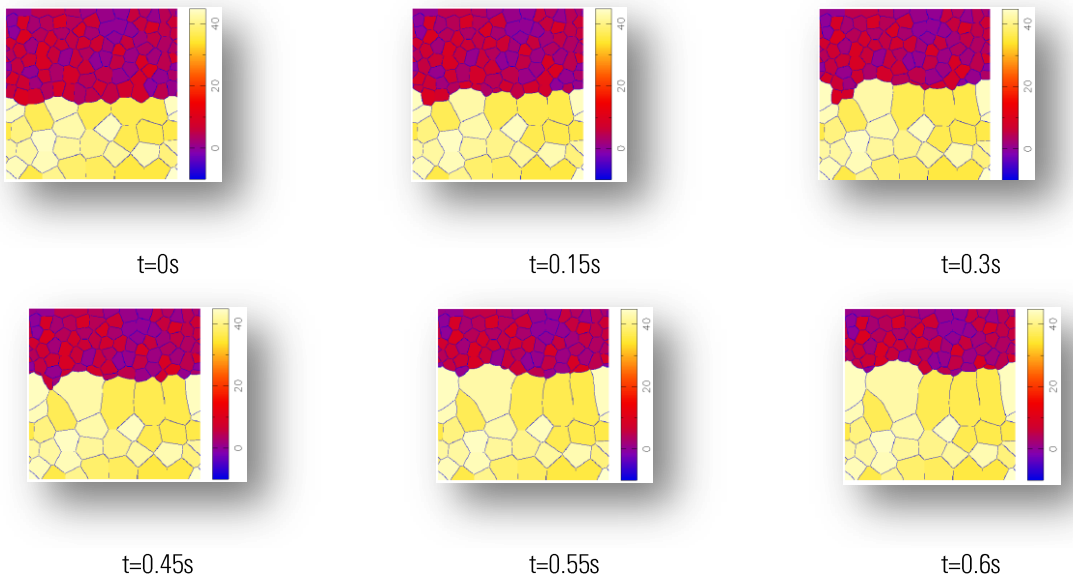


Figure 7. The recrystallisation path: Rex_3_orie.mcr. Different grains may also be distinguished by their orientation

9.3.4 ReX_4_in.txt

- Recrystallisation path presented by the .orie-output

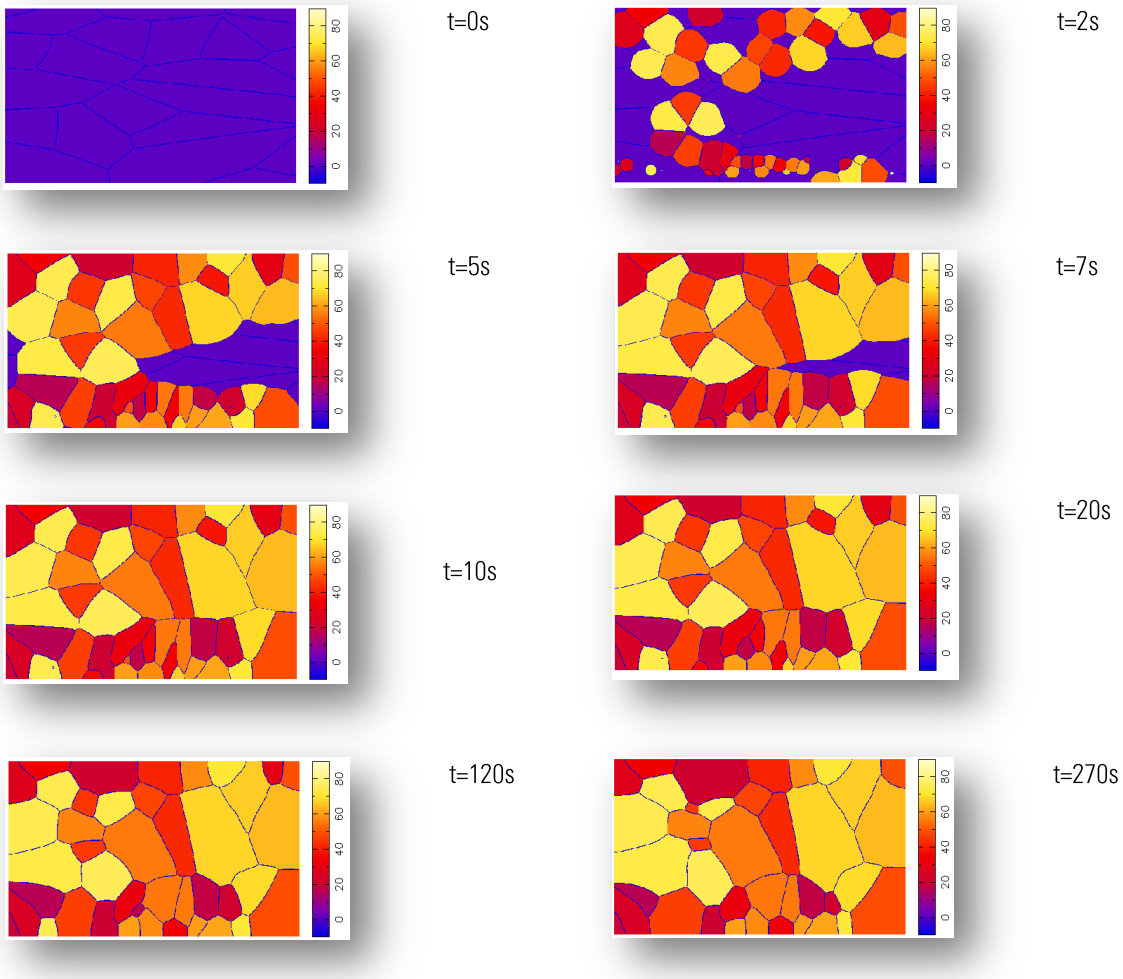


Figure 9.5. The recrystallisation path: Rex_4_orie.mcr

9.3.5 ReX_5_in.txt

- Recrystallisation path presented by the .orie-output

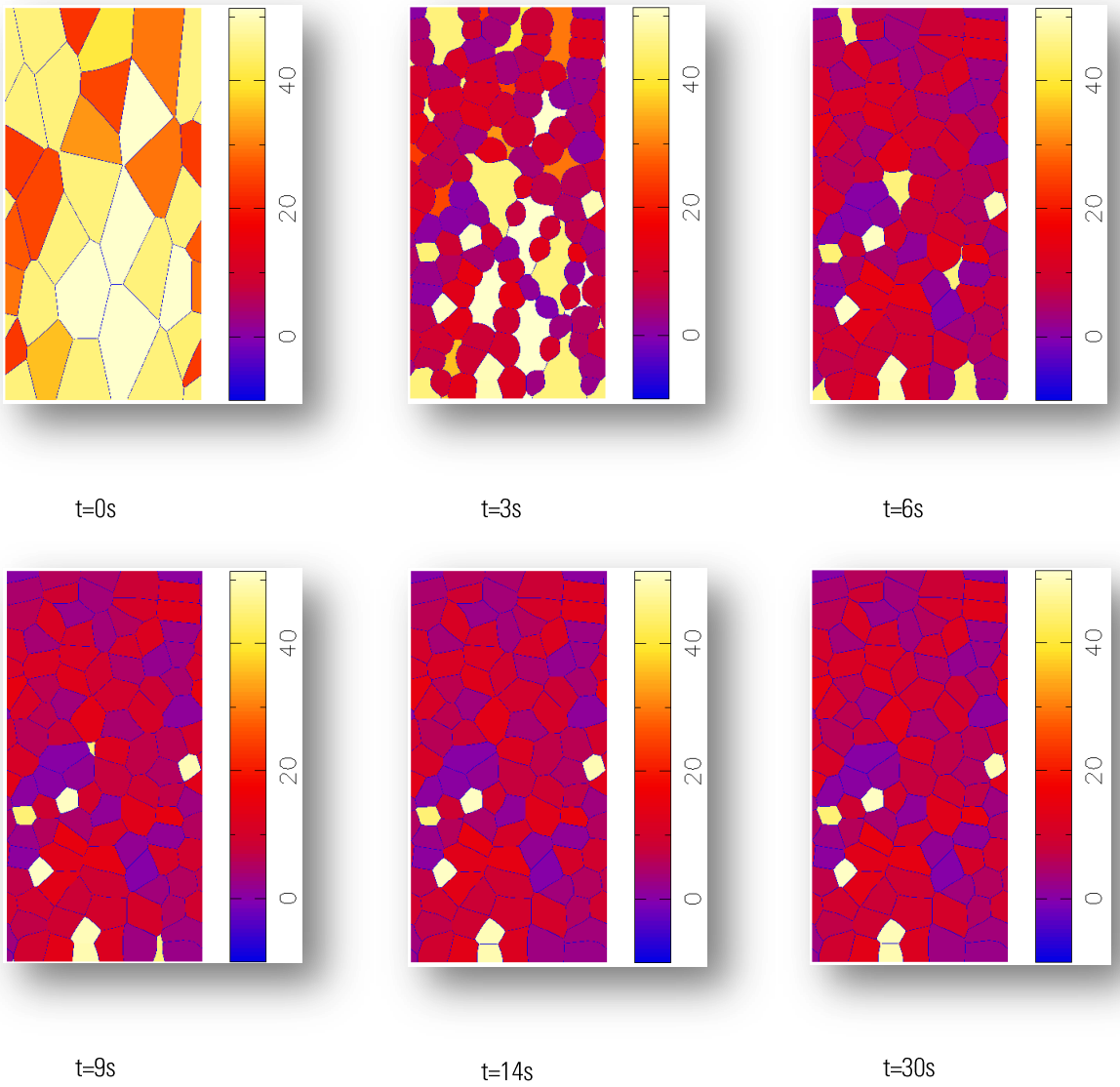


Figure 9.6. The recrystallisation path: Rex_5_orie.mcr

10 "Stress"

10.1 Description

The example "Stress_dri" is concentration-coupled and shows the simulation of Eshelby's solution.

name dri file	Stress_in.txt
alloy system	Fe-C-Mn
composition	0,103 wt% C in austenite 0,49 wt% Mn in austenite
transition	austenite to ferrite (with stress)

Table 14 Example: "Stress":- details

10.2 Simulation conditions

name dri file	Stress_in.txt
dimension	2D
grid size	200x200 cells
grid spacing	0.25μm
interface thickness	5.5 cells
boundary conditions BCs phase field BCs	East: insulation West: insulation bottom: insulation top: insulation
concentration field BCs	East: insulation West: insulation bottom: insulation top: insulation
solid phases:	2 solid phases: austenite (initial/matrix) and ferrite (growing)
grain input	recrystallisation: NO deterministic placement of one austenite grain (round r = 1000μm position x = 0.0 , z = 0.0) and one ferrite grain (round r = 2.5 μm, x= 25.5, z=24.2) (stabilisation of the grain, no Voronoi construction further nucleation: NO latent heat: NO temperature conditions: T_0=1100K; G = 0 K/cm; dT/dt = 0 K/s phase diagram input: linear notation of eigenstrain: volume
output	files: interface, driving force, concentration, normal stress, von Mises stress, normal displacement times: -> fixed output at 0,01 s -> automatic output
special features	-> concentration coupling, stress calulation -> 1d far field diffusion approximation: NO -> thermodynamic coupling: NO -> moving frame: NO

Table 15 Example 01: Delta-Gamma: field parameters

10.3 Visualisation of the results

- The von Mises stress field presented by the .vM-output

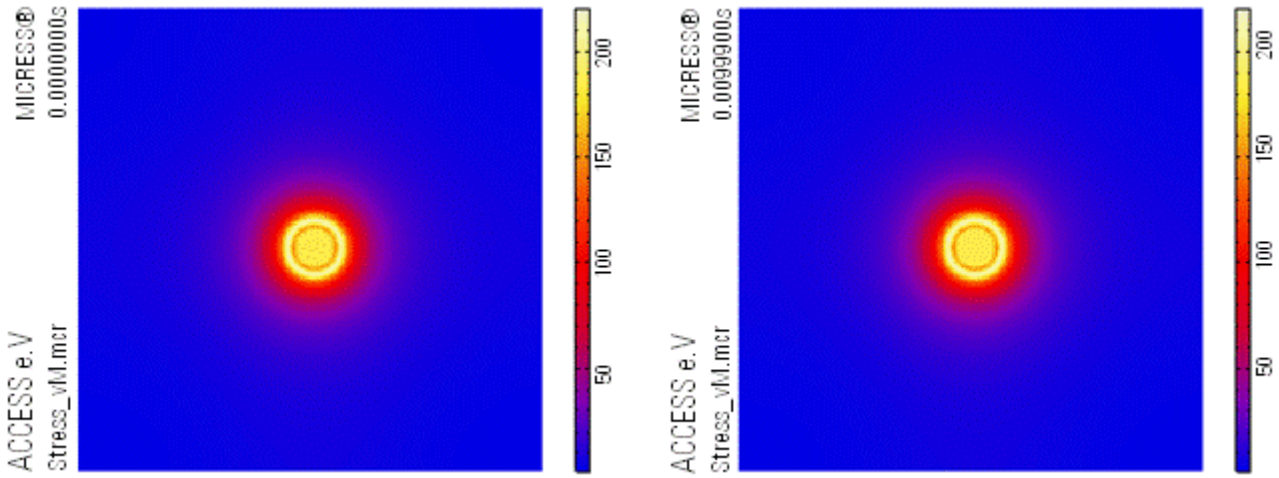
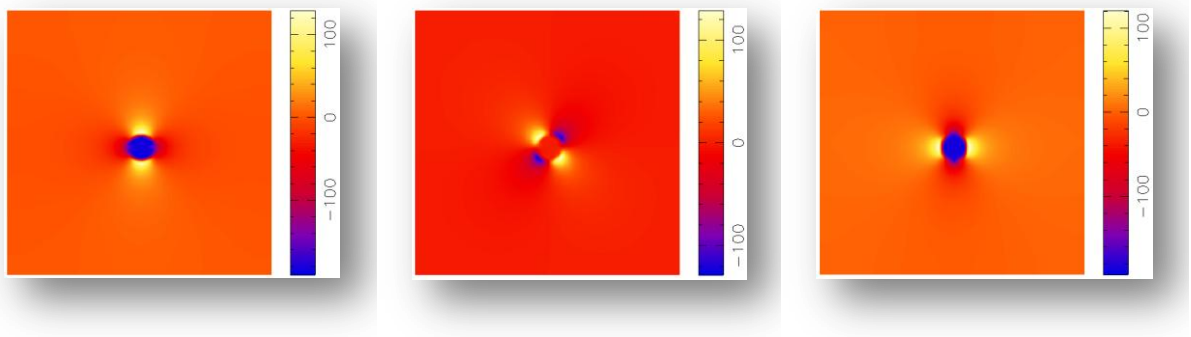


Figure 10.1. The von Mises stress field: Stress_vM.mcr

- Normal stresses in x, y and z-direction presented by the .cV-outputs



t=0s, Stress_sxxCV.mcr t=0s, Stress_sxzCV.mcr t=0s, Stress_szzCV.mcr

Figure 8. The normal stress distributions in different directions

11 "Basic TQ-Coupling"

11.1 Description

The two examples, "TQ_Ripening_dri" and "TQ_Eutectic_dri" illustrate the basics of the Thermo-Calc™ coupling (via its TQ interface). Here, phase transformations are simulated in an aluminium silver alloy. The first model is isothermal and shows the effect of curvature. The second one is similar and adds heat extraction and simulation of latent heat release, with growth of a primary and a secondary phase, as well as solid-solid interaction after the complete solidification.

name dri file	TQ_Ripening_in.txt TQ_Eutectic_in.txt
alloy system	Ag-Al (Seta_Bin.GES5)
composition	32 at% Ag 68 at% Al
transition	phase transformation

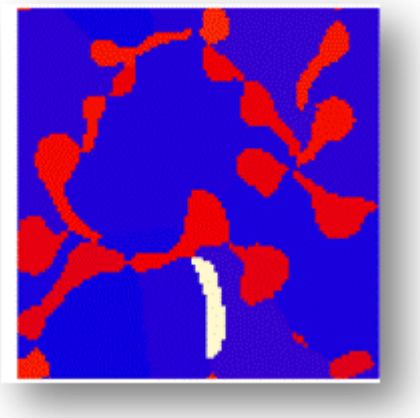


Table 16 Example: "TQ-Coupling":- details

11.2 Simulation conditions

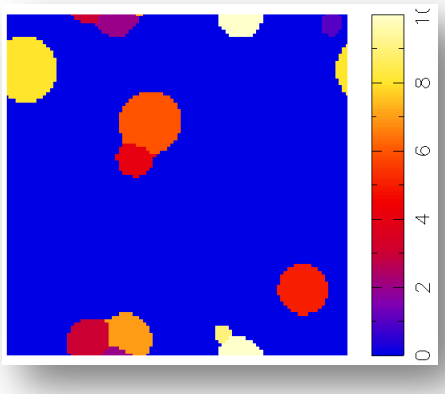
name dri file		TQ_Ripening_in.txt	TQ_Eutectic_in.txt
dimension		2D	
grid size (cells)		100x1x100	
grid spacing		0.1µm	
interface thickness (cells)		4	
boundary conditions BCs			
phase field BCs	East:	periodic	symmetric
	West:	periodic	symmetric
	bottom	periodic	periodic
	top:	periodic	periodic
concentration field BCs	East:	periodic	periodic
	West:	periodic	periodic
	bottom:	periodic	periodic
	top:	periodic	periodic
solid phases:		1 solid phase: FCC_A1	2 solid phases: FCC_A1, HCP_A3
grain input		recrystallisation: NO	
		random placement of grains (round); integer for randomization: 10; stabilisation of the grains; Voronoi construction	
		further nucleation: NO	further nucleation: enabled 1 type of seeds, position of the seeds: interface; maximum number of simultaneous nucleations: 25
		temperature conditions: T_0=845 K; G = 0 K/cm; dT/dt = 0 K/s	
		latent heat: enabled	
output		files: restart, grains, phases, average fraction output, interface output, driving force output, mobility output, curvature, grain-time file, concentration, concentration of the reference phase, linearization output, monitoring outputs	
		times: fixed output at 0.001 s logarithmic step outputs at 1.4142 s and 1 s	times: from 0 s to 0.02 s output every 0.005 s from 0.02 s to 0.55 s output every 0.02 s (linear step)
special features		-> concentration coupling -> NO 1d far field diffusion approximation -> thermodynamic coupling: enabled; Seta_Bin.Ges5 datafile -> NO moving frame	

Table 17 Example: TQ_coupling: field parameters

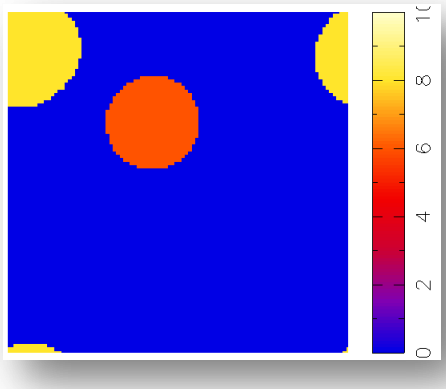
11.3 Visualisation of the results

11.3.1 "TQ_Ripening_in.txt"

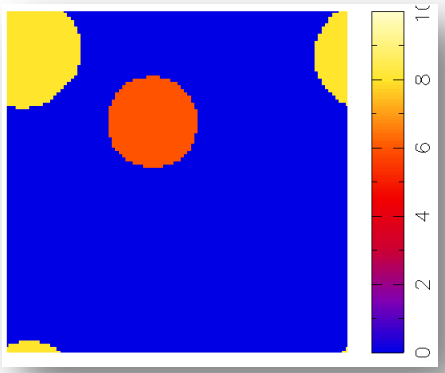
- The ripening sequence presented by the .korn-output (grain numbers)



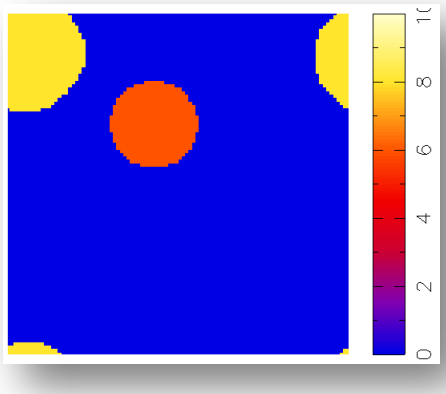
t=0s



t=0.5119116s



t=0.7239454

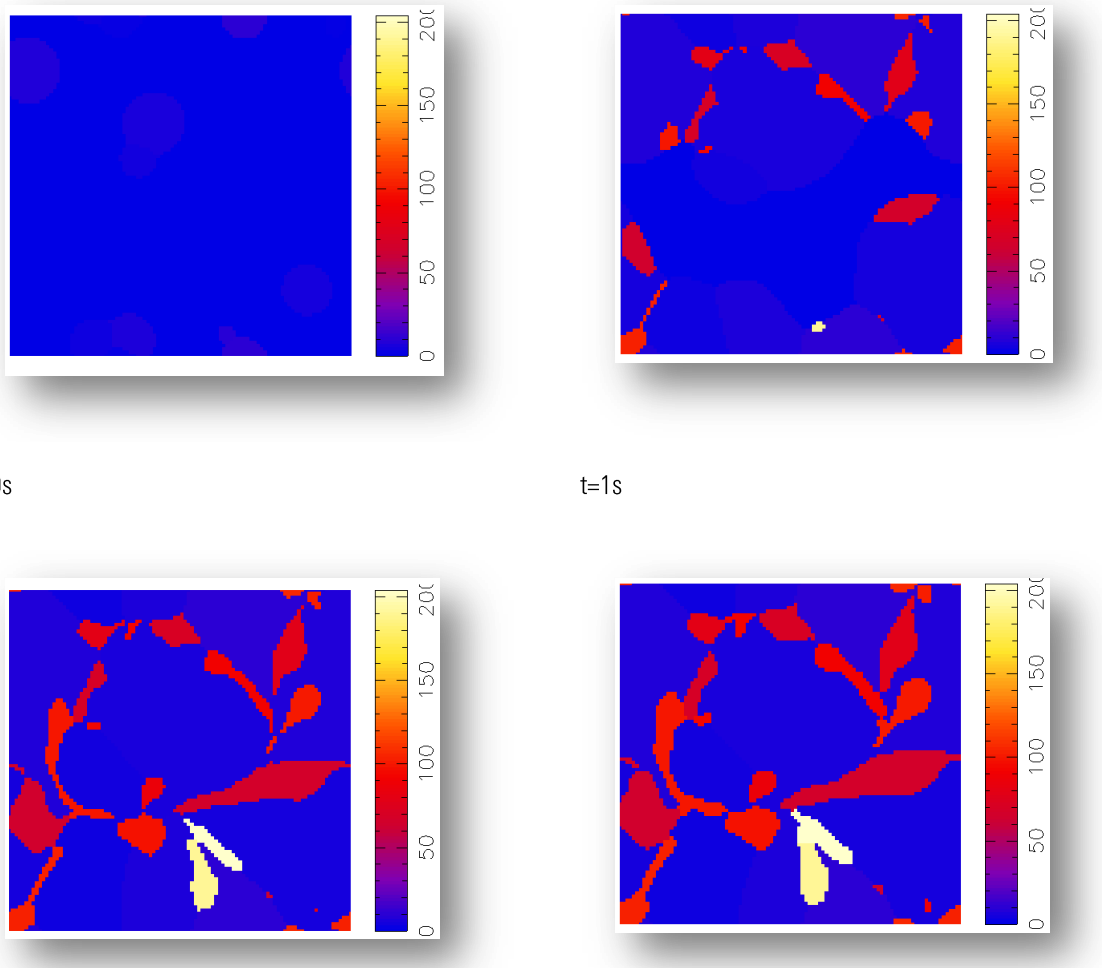


t=1.0s

Figure 11.1. TQ_Ripening_korn.mcr

11.3.2 "TQ_Eutectic_in.txt"

- The phase transition path presented by the .korn-output



t=0s t=1s

t=0.34s t=0.55s

Figure 11.2. TQ_Eutectic_korn.mcr

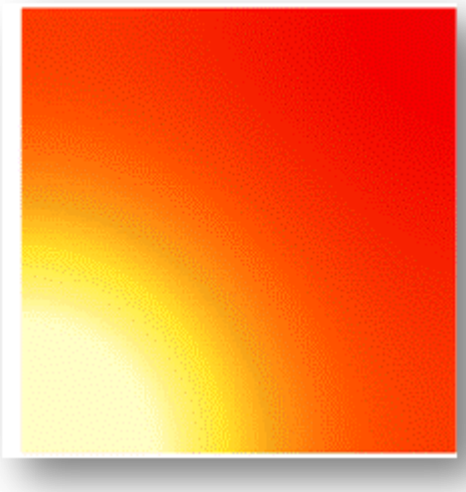
12 "Temperature"

12.1 Description

The example "Temperature_dri" illustrates the use of coupling to a temperature field for the case of a sphere of a pure substance growing into an undercooled liquid.

name dri file	Temperature_in.txt
alloy system	arbitrary model material with Tm = 1000K
composition	pure phase
phenomenon	Solidification of pure substance

Table 18 Example: "Temperature":- details



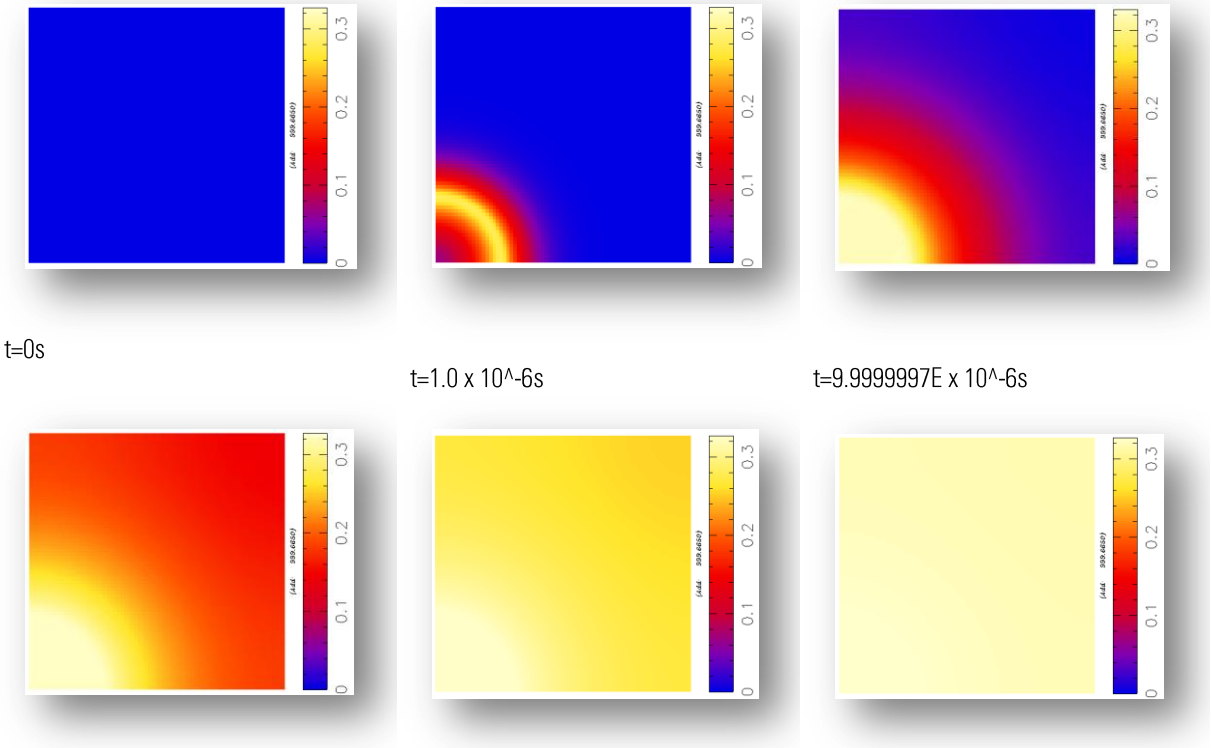
12.2 Simulation conditions

name dri file	Temperature_in.txt
dimension	2D
grid size	75x1x75 cells
grid spacing	1 μm
interface thickness	7 cells
boundary conditions BCs	
phase field BCs	East: insulation West: insulation bottom: insulation top: insulation
temperature field BCs	East: insulation West: insulation bottom: insulation top: insulation
solid phases:	one solid phase (a pure substance)
grain input	recrystallisation: NO deterministic placement of 1 grain (round r = 0,0; position x = 0.0 , z = 0.0; r=20 μm); stabilisation of the grain, Voronoi construction further nucleation: NO temperature conditions: $T_{0,\,bottom}$=999.665 K; $T_{0,\,top}$=999.665 K
output	files: restart data, grain number output, phases, fraction, average fraction table, interface, driving force, mobility, curvature, velocity, grain time file, temperature, monitoring outputs times: -> output at 0,000001 s, 0.00001, 0.00005, 0.0001, 0.0002, 0.002 -> fixed output: time step = 1E-7
special features	-> temperature coupling (gs) -> 1d far field diffusion approximation: NO -> thermodynamic coupling: NO -> moving frame: NO

Table 2: "Temperature" Example: simulation conditions

12.3 Visualisation of the results

- The temperature field as taken from the .temp-output



t=0s | t=1.0 x 10^-6s | t=9.9999997E x 10^-6s

t=4.9999999E x 10^-5s | t=9.9999997E x 10^-5s | t=1.9999999E x 10^-4

Figure 12.1. Temperature_temp.mcr

- Growth of a spherical particle as taken from the .phas-output

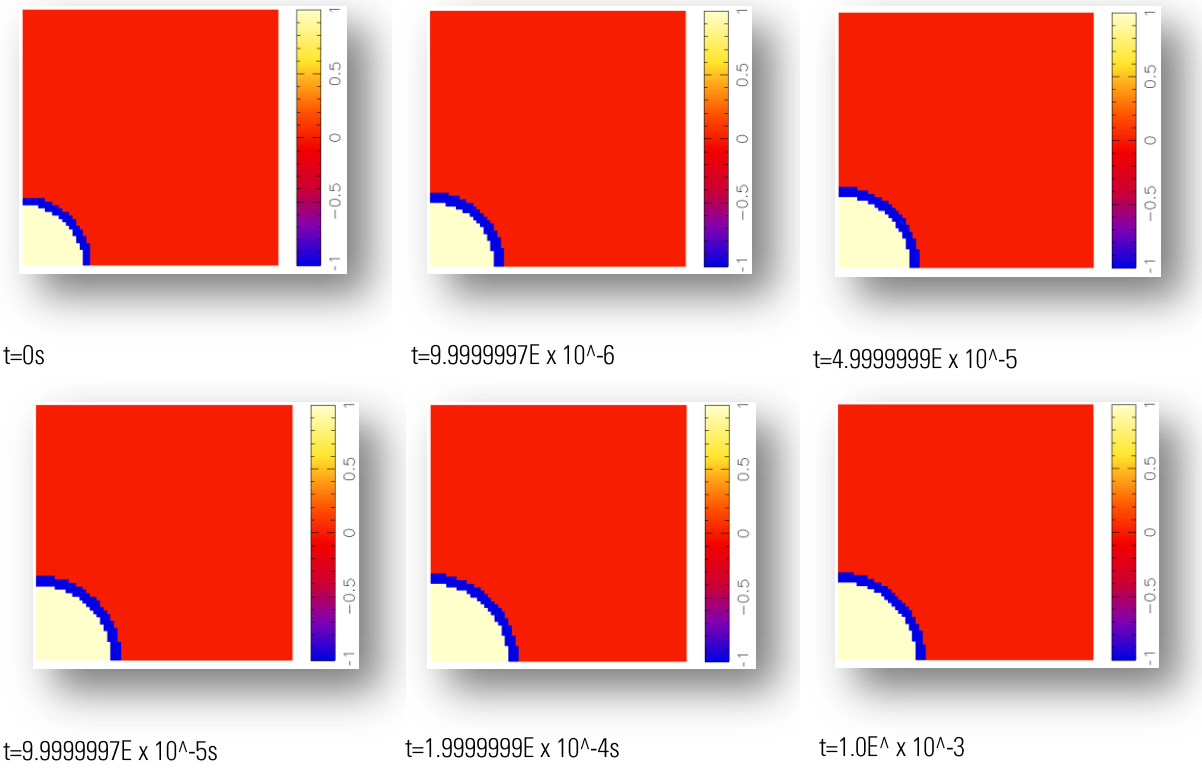


Figure 12.2. Temperature_phas.mcr